TLUSTY User's Guide II: Reference Manual

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Abstract

This is the second part of a three-volume guide to TLUSTY and SYNSPEC. It presents a detailed reference manual for TLUSTY, which contains a detailed description of basic physical assumptions and equations used to model an atmosphere, together with an overview of the numerical methods to solve these equations.

Contents

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1 Introduction

This paper in the second part of a series of three papers that provide a detailed guide to model stellar atmosphere and accretion disk program TLUSTY, and associated spectrum synthesis program SYNSPEC. The first paper (Hubeny & Lanz 2017a; hereafter referred to as Paper I) provides a brief introductory guide to these programs, without much description of the underlying physical, mathematical, and numerical background.

The aim of this paper is to provide just that. We shall summarize the basic structural equations of the problem, and outline the adopted numerical methods to solve the resulting equations. An outline of the actual operation of TLUSTY, and a detailed explanation and description of the input parameters, the individual computational strategies, and various tricks to solve potential numerical problems, is covered in the subsequent Paper III (Hubeny & Lanz 2017c).

A detailed description of the original version of TLUSTY is given by Hubeny (1988). That paper describes the basic concepts, equations, and numerical methods used. However, because the program has evolved considerably since 1988, the description presented in that paper has become in many places obsolete. The major new developments are described in several papers: Hubeny & Lanz (1992) presented the Ng and Kantorovich accelerations; Hubeny & Lanz (1995) developed the hybrid CL/ALI method, and the concept of superlevels and superlines treated by means of an Opacity Distribution Functions (ODF) or Opacity Sampling (OS). A treatment of level dissolution, occupation probabilities, merged levels, and corresponding pseudocontinuum is described by Hubeny, Hummer, & Lanz (1994). An extension to high-temperature conditions, including Compton scattering, X-ray opacities with inner-shell (Auger) ionization, is described in Hubeny et al. (2001). A general and comprehensive overview of the physical and mathematical formulation of the problem is presented in Hubeny & Mihalas (2014; Chaps.12, 13, 14, 17, 18).

2 Physical background

TLUSTY is designed to compute the so-called classical model atmospheres; that is, plane-parallel, horizontally homogeneous atmospheres in hydrostatic and radiative (or radiative+convective) equilibrium. For a comprehensive discussion and detailed description of the basic physics and numerics of the problem, refer to Hubeny & Mihalas (2014; Chap. 18).

In the next section, we describe the basic assumptions and structural equations specific to stellar atmospheres. The equations are generally non-local and therefore depend on the geometry of the problem. Analogous assumptions and equations for accretion disks will be described in the subsequent section, while the local physics and corresponding equations, valid for both atmospheres and disks, will be covered in the rest of the chapter.

2.1 Basic equations of stellar atmospheres

• Radiative transfer equation

It is convenient to use the second-order form

$$\frac{d^2(f_\nu J_\nu)}{d\tau_\nu^2} = J_\nu - S_\nu, \tag{1}$$

where f_ν is the variable Eddington factor, J_ν the mean intensity of radiation at frequency ν, τ_ν the monochromatic optical depth and S_ν the source function, defined by

$$S_\nu = \eta_\nu^{\text{tot}}/\chi_\nu, \tag{2}$$

where χ_ν is the total absorption coefficient, and η_ν^{tot} the total emission coefficient. The Eddington factor is defined by

$$f_\nu \equiv K_\nu/J_\nu = \int_{-1}^{1} I_\nu(\mu)\mu^2\, d\mu \Big/ \int_{-1}^{1} I_\nu(\mu)\, d\mu, \tag{3}$$

where $\mu = \cos\theta$, with θ being the angle between the direction of propagation of the radiation and the normal to the surface. The optical depth is defined by

$$d\tau_\nu \equiv -\chi_\nu dz = (\chi_\nu/\rho)\, dm, \tag{4}$$

where z is a geometrical distance measured along the normal to the surface from the bottom of the atmosphere to the top, m the column mass, and ρ the mass density – see equation (12). The column mass is taken as the basic geometrical coordinate.

The upper boundary condition is written as

$$\left[\frac{\partial(f_\nu J_\nu)}{\partial\tau_\nu}\right]_0 = g_\nu J_\nu(0) - H_\nu^{\text{ext}}, \tag{5}$$

where g_ν is the surface Eddington factor defined by

$$g_\nu \equiv \frac{1}{2}\int_{-1}^{1} I_\nu(\mu,0)\mu\, d\mu / J_\nu(0), \tag{6}$$

and

$$H_\nu^{\text{ext}} \equiv \frac{1}{2}\int_0^1 I_\nu^{\text{ext}}(\mu)\mu\, d\mu \tag{7}$$

where $I_\nu^{\text{ext}}(\mu)$ is an external incoming intensity at the top of the atmosphere. In most cases one assumes no incoming radiation, $I_\nu^{\text{ext}}(\mu) = 0$, but can be taken as a non-zero input quantity if needed.

The lower boundary condition is written in a similar way

$$\left[\frac{\partial(f_\nu J_\nu)}{\partial\tau_\nu}\right]_{\tau_{\text{max}}} = H_\nu^+ - \frac{1}{2}J_\nu, \tag{8}$$

where $H_\nu^+ = \frac{1}{2} \int I_\nu^+(\mu, \tau_{\max}) \mu\, d\mu$. One typically assumes the diffusion approximation at the lower boundary, in which case $I_\nu^+(\mu) = B_\nu + \mu(dB_\nu/d\tau_\nu)$, hence equation (8) is written as

$$\left[\frac{\partial(f_\nu J_\nu)}{\partial \tau_\nu} \right]_{\tau_{\max}} = \left[\frac{1}{2}(B_\nu - J_\nu) + \frac{1}{3}\frac{\partial B_\nu}{\partial \tau_\nu} \right]_{\tau_{\max}}, \tag{9}$$

where B_ν is the Planck function,

$$B_\nu = \frac{2h\nu^3}{c^2} \frac{1}{\exp(h\nu/kT) - 1}, \tag{10}$$

where T is the temperature, and h, k, c are the Planck constant, Boltzmann constant, and the speed of light, respectively.

Equations (1), (5), and (9) contain only the mean intensity of radiation, J_ν, a function of frequency and depth, but not the specific intensity, $I_{\mu\nu}$, which is also a function of the polar angle θ ($\mu = \cos\theta$). This is made possible by introducing the Eddington factor, which is computed in the formal solution of the transfer equation, and is held fixed during the subsequent iteration of the linearization process. By the term "formal solution" we mean a solution of the transfer equation with *known* source function. It is done between two consecutive iterations of the iterative scheme, with the current values of the state parameters – see § 3.8.

• Hydrostatic equilibrium equation

The equation is conveniently written as

$$\frac{dP}{dm} = g, \tag{11}$$

where P is the total (gas plus radiation) pressure, and m the Lagrangian mass, or column mass,

$$dm = -\rho\, dz, \tag{12}$$

g is the surface gravity, which is assumed constant throughout the atmosphere, and given by $g = GM_*/R_*^2$, where M_* and R_* are the stellar mass and radius, respectively; G is the gravitational constant. The surface gravity g is one of the basic parameters of the problem.

The total pressure is generally composed of three parts, the gas pressure, P_{gas}, the radiation pressure, P_{rad}, and a "turbulent pressure", P_{turb}. The gas pressure is given, assuming an ideal gas equation of state, by

$$P_{\text{gas}} = NkT, \tag{13}$$

where T is the (electron) temperature, and N is the total particle number density. The radiation pressure is given by

$$P_{\text{rad}} = \frac{4\pi}{c} \int_0^\infty K_\nu d\nu. \tag{14}$$

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The so-called "turbulent pressure" is not a well-defined quantity; it is introduced to mimic a pressure associated with a random motion of "turbulent eddies" as $P_{\text{turb}} \propto \rho v_{\text{turb}}^2$, where v_{turb} is the microturbulent velocity. It can be included in TLUSTY model calculations, but it is not recommended since its physical meaning is questionable.

The hydrostatic equilibrium equation can then be written as

$$\frac{d(P_{\text{gas}} + P_{\text{turb}})}{dm} = g - \frac{4\pi}{c} \int_0^\infty \frac{dK_\nu}{dm}\, d\nu = g - \frac{4\pi}{c} \int_0^\infty \frac{\chi_\nu}{\rho} H_\nu\, d\nu, \qquad (15)$$

where H_ν and K_ν are the first and second angular moments of the specific intensity.

● Energy balance equation

In the convectively stable layers, the energy balance is represented by the radiative equilibrium equation. For the purposes of numerical stability, it is considered in TLUSTY as a linear combination of its two possible forms – the terms in square brackets of equation (16), that both should be identically equal to zero,

$$\alpha \left[\int_0^\infty \left(\chi_\nu J_\nu - \eta_\nu^{\text{tot}} \right) d\nu \right] + \beta \left[\int_0^\infty \frac{d(f_\nu J_\nu)}{d\tau_\nu}\, d\nu - \frac{\sigma_R}{4\pi} T_{\text{eff}}^4 \right] = 0, \qquad (16)$$

where α and β are empirical coefficients that satisfy $\alpha \to 1$ in the upper layers, and $\alpha \to 0$ for deep layers, while the opposite applies for β. The division between the "surface" and "deep" layers is a free parameter. In equation (16), σ_R is the Stefan-Boltzmann constant and T_{eff} the effective temperature, which is a measure of the total energy flux coming from the interior. It is another basic parameter of the problem.

The first term of equation (16) is called the "integral form", while the second the "differential" form. Using Eqs. (86) and (89), and assuming coherent scattering in the scattering part of the emission coefficient, the integral form may be rewritten in a traditional form

$$\int_0^\infty \left(\chi_\nu J_\nu - \eta_\nu^{\text{tot}} \right) d\nu = \int_0^\infty \left(\kappa_\nu J_\nu - \eta_\nu \right) d\nu, \qquad (17)$$

where κ_ν and η_ν are the extinction and thermal emission coefficients, respectively.

● Convection

The atmosphere is convectively unstable if the Schwarzschild criterion for convective instability is satisfied,

$$\nabla_{\text{rad}} > \nabla_{\text{ad}}, \qquad (18)$$

where $\nabla_{\text{rad}} = (d\ln T / d\ln P)_{\text{rad}}$ is the logarithmic temperature gradient in radiative equilibrium, and ∇_{ad} is the adiabatic gradient. The latter is viewed as

a function of temperature and pressure, $\nabla_{\mathrm{ad}} = \nabla_{\mathrm{ad}}(T,P)$. The density ρ is considered to be a function of T and P through the equation of state.

If convection is present, equation (16) is modified to read

$$\alpha\left[\int_0^\infty (\kappa_\nu J_\nu - \eta_\nu)\,d\nu + \frac{\rho}{4\pi}\frac{dF_{\mathrm{conv}}}{dm}\right] + \beta\left[\int_0^\infty \frac{d(f_\nu J_\nu)}{d\tau_\nu}\,d\nu - \frac{\sigma_R}{4\pi}T_{\mathrm{eff}}^4 + \frac{F_{\mathrm{conv}}}{4\pi}\right] = 0 \tag{19}$$

where F_{conv} is the convective flux, given by

$$F_{\mathrm{conv}} = (gQH_P/32)^{1/2}(\rho c_P T)(\nabla - \nabla_{\mathrm{el}})^{3/2}(\ell/H_P)^2, \tag{20}$$

where $H_P \equiv -(d\ln P/dz)^{-1} = P/(\rho g)$ is the pressure scale height, c_P is the specific heat at constant pressure, $Q \equiv -(d\ln\rho/d\ln T)_P$, and ℓ/H_P is the ratio of the convective mixing length to the pressure scale height, taken as a free parameter of the problem, ∇ is the actual logarithmic temperature gradient, and ∇_{el} is the gradient of the convective elements. The latter is determined by considering the efficiency of the convective transport; see, e.g., Hubeny and Mihalas (2014; § 16.5),

$$\nabla - \nabla_{\mathrm{el}} = (\nabla - \nabla_{\mathrm{ad}}) + B^2/2 - B\sqrt{B^2/2 - (\nabla - \nabla_{\mathrm{ad}})}, \tag{21}$$

where

$$B = \frac{12\sqrt{2}\sigma_R T^3}{\rho c_p (gQH_P)^{1/2}(\ell/H_P)}\frac{\tau_{\mathrm{el}}}{1 + \tau_{\mathrm{el}}^2/2}, \tag{22}$$

with $\tau_{\mathrm{el}} = \chi_R\ell$ is the optical thickness of the characteristic element size ℓ. The gradient of the convective elements is then a function of temperature, pressure, the actual gradient, $\nabla_{\mathrm{el}} = \nabla_{\mathrm{el}}(T,P,\nabla)$, and the convective flux can also be regarded as a function of T, P, and ∇.

For white dwarfs, Fontaine et al. (1992) suggested a slightly different prescription for the convective flux, called ML2, which essentially consists of replacing the factor $\sqrt{1/32}$ in Eq. (20) by 2. This possibility is also offered by TLUSTY.

● Other structural equations

The rest of structural equations, namely the kinetic equilibrium equation, charge and particle conservation equation, equation of state, together with auxiliary equations such as the definition of absorption and emission coefficients, are local, and therefore the same for stellar atmospheres and accretion disks, and will be described in §§ 2.3 - 2.4.

2.2   Accretion disks

The basic assumptions are the following:

- The disk is divided into a set of concentric rings, each behaving as an independent 1-D plane parallel radiating slab; no assumptions about optical thickness are made. One run of TLUSTY calculates a vertical structure of one ring;

- hydrostatic equilibrium in the vertical z-direction;

- energy balance is considered as a balance between the net radiation loss (calculated exactly, without invoking neither optically thin, nor optically thick [diffusion] approximations), and the mechanical energy generated through viscous dissipation;

- the dissipated energy is proportional to viscosity, which is given through the empirical viscosity parameter α or through a Reynolds number;

One can consider accretion disks around stars – the so-call *classical disks*, in which case the basic radial structure is given by the standard model (e.g., Frank, King, Raine 1992), or disks around black holes – the so-called *relativistic disks*, in which case the radial structure is given essentially by Novikov & Thorne (1973), with refinements described in Riffert & Herold (1995) and Krolik (1999). We use a universal formalism, in which case the relativistic disks are described by means of *relativistic corrections*. We follow the notation of Riffert & Herold (1995) and Hubeny & Hubeny (1998).

2.2.1 General structural equations

The basic structural equations for one individual ring are the following:

• Vertical hydrostatic equilibrium equation

The atmosphere at each disk radius R (specified in the disk midplane) is in hydrostatic equilibrium, with a depth-dependent gravity (g) that arises from the vertical component of the central star's gravitational force on the disk material. Neglecting the self-gravity of the disk and assuming that R is much larger than the distance from the central plane, z:

$$\frac{dP}{dz} = -g(z)\rho, \quad \text{or} \quad \frac{dP}{dm} = g(z), \tag{23}$$

where the depth-dependent vertical gravity acceleration is given by

$$g(z) = \frac{GM}{R^3} \frac{C}{B} \, z \,. \tag{24}$$

G is the gravitational constant, M is the mass of the central object, and B and C (together with A used later) are the so-called relativistic corrections in the notation of Riffert and Harold (1995). For classical disks, $A = B = C = 1$.

• Energy balance

Generally, it is written as

$$\frac{\partial F_z}{\partial z} = \frac{3}{2} \left(\frac{GM}{R^3} \right)^{1/2} \frac{A}{B} \, t_{\phi r}, \tag{25}$$

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where F_z is the z-component of the energy flux and $T_{\phi r}$ is the sheer stress, also called the viscous stress.

• Azimuthal momentum balance

Under the assumption of $t_{\phi r} = 0$ at the innermost orbit, it is written as

$$\int_{-h}^{h} t_{\phi r} dz = \frac{\dot{M}}{2\pi} \left(\frac{GM}{R^3} \right)^{1/2} \frac{D}{A},\tag{26}$$

where h is the vertical height of the given annulus, and $\dot{M}$ is the mass accretion rate.

• Equation describing the source of viscous stress

$$t_{\phi r} = \frac{3}{2}\eta \left(\frac{GM}{R^3} \right)^{1/2} \frac{A}{B},\tag{27}$$

where η is the coefficient of sheer viscosity, which is expressed through the coefficient of kinematic viscosity w as $\eta \equiv \rho w$.

• The coefficients A - D are given by:

For classical disks,

$$A = B = C = 1,\tag{28}$$
$$D = 1 - (R/R_*)^{1/2},\tag{29}$$

where R_* is the radius of the central star.

For relativistic disks, they are called the relativistic corrections:

$$A = 1 - \frac{2}{r} + \frac{a^2}{r^2},\tag{30}$$

$$B = 1 - \frac{3}{r} + \frac{2a}{r^{3/2}},\tag{31}$$

$$C = 1 - \frac{4a}{r^{3/2}} + \frac{3a^2}{r^2},\tag{32}$$

$$D = \frac{1}{\sqrt{r}} \int_{r_i}^{r} \frac{x^2 - 6x + 8a\sqrt{x} - 3a^2}{\sqrt{x}(x^2 - 3x + 2a\sqrt{x})} dx,\tag{33}$$

where r is the radius of the annulus is expressed in units of the gravitational radius, $r = R/(GM/c^2)$, and a is the specific angular momentum (spin) of the black hole expressed in units of G/c ($a = 0$ for a Schwarzschild black hole; $a = 0.998$ for maximum rotating Kerr black hole).

2.2.2   Viscosity and the total column mass

To write down practical expressions of the energy balance and for the total column mass, one has to introduce a suitable parametrization of viscosity. First, the sheer viscosity η is expressed through the kinematic viscosity w as

$$\eta \equiv \rho w.\tag{34}$$

The corresponding vertically averaged kinematic viscosity is given by

$$\bar{w} = \frac{\int_0^h w\rho dz}{\int_0^h \rho dz} = \frac{1}{m_0} \int_0^h \eta dz = \frac{1}{m_0} \int_0^{m_0} w\, dm. \tag{35}$$

Integrating Eq. (27) from 0 to h, and using Eq. (26) together with Eq. (35), one can express the total column mass at the midplane through the averaged viscosity as

$$m_0 = \frac{1}{\bar{w}} \frac{\dot{M}}{6\pi} \frac{BD}{A^2}, \tag{36}$$

There are two possibilities to express the viscosity. A simple one is to parametrize it through the Reynolds number (Lynden-Bell & Pringle 1974, Kříž & Hubeny 1986), in which case the vertically averaged viscosity is simply given as

$$\bar{w} = \frac{(GMR)^{1/2}}{\text{Re}}, \tag{37}$$

where Re is the Reynolds number, which is a free parameter of the problem, typically chosen between 1000 and 10000 (Lynden-Bell & Pringle 1974). Consequently, the total column mass m_0 is simply

$$m_0 = \frac{\dot{M}\text{Re}}{6\pi(GMR)^{1/2}} \frac{BD}{A^2}, \tag{38}$$

which has a big computational advantage that m_0 is given as a function of M, $\dot{M}$, and R (and the spin a in the case of relativistic disks), and therefore is known a priori. However, it is not clear how to choose a proper value of the Reynolds number and, moreover, whether the same Reynolds number applies for all radial distances in a disk.

Therefore, a much more commonly used prescription is based on the so-called α-parametrization (Shakura & Sunyaev 1973). There are several variants of this parametrization; we use here a version in which the vertically averaged sheer viscosity is taken proportional to the vertically averaged (total) pressure,

$$\bar{t_{\phi r}} \equiv \frac{1}{h} \int_0^h t_{\phi r} dz = \alpha \bar{P}, \tag{39}$$

in which case

$$\int_0^h t_{\phi r} dz = h\alpha \bar{P} = m_0 \alpha (\bar{P}/\bar{\rho}), \tag{40}$$

where the averaged density is given by $\bar{\rho} = m_0/h$. The vertically averaged kinematic viscosity is given by substituting Eqs. (27) integrated over z into Eq. (40),

$$\bar{w} = \alpha \frac{2}{3} \left(\frac{R^3}{GM} \right)^{1/2} \frac{B}{A} \left(\frac{\bar{P}}{\bar{\rho}} \right). \tag{41}$$

A disadvantage of the α-prescription is that the vertically averaged kinematic viscosity, and the total column mass are not known a priori since they depend on $(\bar{P}/\bar{\rho})$, which can only be accurately computed when the model is constructed.

In the case of dominant radiation pressure, one can, however, derive a relation between $\bar{P}$ and $\bar{\rho}$ prior to solving for the detailed structure (e.g., Hubeny & Hubeny 1998). In this case, the vertically-averaged kinematic viscosity is given through α as

$$\bar{w} = 2\dot{M}^2\alpha \left(\frac{GM}{R^3}\right)^{1/2} \left(\frac{\sigma_{\mathrm{e}}}{8\pi m_H c}\right)^2 \frac{D^2}{AC}, \qquad (42)$$

and, with the α-parametrization of viscosity, the total column mass is given by

$$m_0 = \frac{16\pi}{3} \left(\frac{m_H c}{\sigma_{\mathrm{e}}}\right)^2 \left(\frac{R^3}{GM}\right)^{1/2} \frac{1}{\dot{M}\alpha} \frac{BC}{AD}, \qquad (43)$$

In the case where the radiation pressure is not dominant, the (approximate) relation between the total column mass m_0 and the viscosity parameter α is given by

$$\alpha m_0 \left(a + \beta m_0^{1/4}\right) - \gamma = 0. \qquad (44)$$

where

$$a = (\sigma_R T_{\mathrm{eff}}^4 \chi_{\mathrm{e}}/c)^2/(3Q), \qquad (45)$$

$$\beta = 0.8 R_g \, \kappa_0^{1/8} (2Q/\pi R_g)^{1/16} T_{\mathrm{eff}}^{1/2}, \qquad (46)$$

and

$$\gamma = (\dot{M}/4\pi)(GM/R^3)^{1/2}(D/A), \qquad (47)$$

where $R_g = 1.3 \times 10^8$ is the gas constant, $\chi_{\mathrm{e}} = \sigma_{\mathrm{e}}/m_H = 0.39$, and $\kappa_0 = 6.4 \times 10^{24}$ is the coefficient in the Kramers-type expression for the Rosseland mean opacity,

$$\kappa_R \approx \kappa_0 \rho T^{-7/2}. \qquad (48)$$

Equation (44) follows from Eqs. (26) and (40), where one makes an approximation that

$$(\bar{P}/\bar{\rho}) \approx (\bar{P}/\bar{\rho})_{\mathrm{rad}} + (\bar{P}/\bar{\rho})_{\mathrm{gas}}, \qquad (49)$$

where $(\bar{P}/\bar{\rho})_{\mathrm{rad}}$ and $(\bar{P}/\bar{\rho})_{\mathrm{gas}}$ correspond to the radiation-pressure dominated and gas-pressure dominated situation, respectively.

The non-linear equation (44) for m_0 is solved by the Newton-Raphson method. In the case of negligible gas pressure we have $\beta m_0^{1/4} \ll a$, so Eq. (44) becomes a simple linear equation for m_0. It can be easily verified that its solution is identical to that given by Eq. (43).

● Parametrization of the local viscosity

The (depth-dependent) viscosity w is allowed to vary as a step-wise power law of the mass column density, viz.

$$w(m) = w_0 \left(m/m_0\right)^{\zeta_0}, \quad m > m_{\mathrm{d}}, \qquad (50)$$

$$w(m) = w_1 \, (m/m_0)^{\zeta_1} \, , \quad m < m_\mathrm{d} \, , \tag{51}$$

where m_d is the division point. In other words, we allow for a different power-law exponent for inner and outer layers, and also for a different portion of the total energy dissipated in these layers. This represents a generalization of an approach we used previously, based on a single power-law representation. For details, refer to Paper III, § 12.8.

We stress that this parametrization is an empirical one. The most natural way of treating local viscosity would be to keep the coefficient of kinematic viscosity constant with depth, i.e., $\zeta_0 = \zeta_1 = 0$. We have originally introduced a power-law parametrization to avoid numerical problems at the surface (Kříž & Hubeny 1986), where $\zeta_1 > 0$. One can also simulate a dissipation that occurs preferentially at the surface layers, with viscosity increasing with decreasing depth which leads to the formation of a disk corona. In this case one choses $\zeta_1 < 0$. Parameter ζ_0 is typically taken as 0.

2.2.3 Actual form of structural equations to be solved

As in the case of stellar atmospheres, the basic geometrical coordinate is the column mass, m. The above structural equations, supplemented by the radiative transfer equation, are written as follows:

• Radiative transfer equation

This equation, and its upper boundary condition, is exactly the same as for stellar atmospheres, equations (1) and (8); the only difference is the lower boundary condition that represents a symmetry condition at the midplane,

$$H_\nu = 0, \quad \text{or} \quad \frac{d(f_\nu J_\nu)}{d\tau_\nu} = 0. \tag{52}$$

• Vertical hydrostatic equilibrium equation

Equations (23), using Eq. (24) is rewritten as

$$\frac{dP}{dm} = Qz, \tag{53}$$

where

$$Q \equiv \frac{GM}{R^3} \frac{C}{B}. \tag{54}$$

• Energy balance

Integrating Eq. (25) over z, and using Eq. (26), one obtains for the total energy flux at the surface which is expressed, in analogy to stellar atmospheres, through the effective temperature,

$$F_z(h) \equiv \sigma_R T_\mathrm{eff}^4 \;=\; \frac{3}{8\pi} \frac{GM\dot{M}}{R^3} \frac{D}{B} \, , \tag{55}$$

The integral form of the energy balance equation follows directly from Eqs. (25), (27), and (34):

$$4\pi \int_0^\infty (\eta_\nu - \kappa_\nu J_\nu) d\nu = \frac{9}{4} \frac{GM}{R^3} \left(\frac{A}{B}\right)^2 \rho w, \tag{56}$$

where the left-hand side, analogous to the case of stellar atmospheres, expresses the net energy radiated away from the unit volume, while the right-hand side expresses the total energy generated by viscous dissipation in the same unit volume. The differential form, in analogy with the atmospheric case, is written as:

$$4\pi \int_0^\infty \frac{d(f_\nu J_\nu)}{d\tau_\nu} d\nu = \sigma_R T_{\text{eff}}^4 [1 - \theta(m)], \tag{57}$$

where the function θ is defined by

$$\theta(m) \equiv \frac{1}{\bar{m}_0} \int_0^m w(m') \, dm', \tag{58}$$

which is a monotonically increasing function of m with $\theta(0) = 0$ and $\theta(m_0) = 1$, for any dependence of the local viscosity on depth.

As in the case of stellar atmospheres, one uses here a linear combination of Eqs. (56) and (57). If convection is present, the convective flux is added analogously as in Eq. (19) for stellar atmospheres. The complete energy balance equation then reads:

$$\alpha \left[\int_0^\infty (\kappa_\nu J_\nu - \eta_\nu) \, d\nu + E_{\text{diss}} + \frac{\rho}{4\pi} \frac{dF_{\text{conv}}}{dm} \right] +$$
$$\beta \left[\int_0^\infty \frac{d(f_\nu J_\nu)}{d\tau_\nu} \, d\nu - \frac{\sigma_R}{4\pi} T_{\text{eff}}^4 [1 - \theta(m)] + \frac{F_{\text{conv}}}{4\pi} \right] = 0, \tag{59}$$

where

$$E_{\text{diss}} = \frac{9}{16\pi} \frac{GM}{R^3} \left(\frac{A}{B}\right)^2 \rho w \tag{60}$$

is the total energy generated by viscous dissipation per unit volume.

● z-m relation

Unlike the case of stellar atmospheres, where the vertical coordinate z has no special meaning, for disks it has to be calculated for given column mass and current density because the gravitational acceleration depends on it through equations (23) and (24). The z-m relation, given by Eq. (12) has to be considered as one of the structural equations.

● Other structural equations

The rest of structural equations, namely the kinetic equilibrium equations for explicit levels, equation of state, and charge conservation equation, together with auxiliary equations such as the definition of absorption and emission coefficients, are local, and therefore the same as in the case of stellar atmospheres.

Table 1: Comparison of stellar atmospheres and accretion disks

Stellar atmospheres	Accretion disks
radiative equilibrium: $\int(\eta_\nu - \kappa_\nu J_\nu)d\nu = 0$	no radiative equilibrium: $\int(\eta_\nu - \kappa_\nu J_\nu)d\nu = E_{\text{diss}}$
g constant	$g = Qz$ (dependent on vertical distance)
$\tau_{\text{tot}} \to \infty$	τ_{tot} finite; not a priori known
Lower boundary: diffusion approx.	Lower boundary: symmetry
Basic parameters: T_{eff}, g, $[A]$	Basic parameters: T_{eff}, Q, m_0, $[A]$

Here, E_{diss} is the dissipated energy given by Eq. (60), Q is the gravity acceleration parameter given by Eq. (54), τ_{tot} denotes any optical depth (monochromatic or mean) at the midplane, and $[A]$ denotes a collection of chemical abundances of all species that are taken into account (see below). The entry "Lower boundary" means the form of the lower boundary condition for the radiative transfer equation. Notice that in the case of disks, the parameters T_{eff}, Q, m_0 are not the fundamental ones, but are evaluated from the more fundamental parameters that specify the disk and the ring within it, namely M, $\dot{M}$, R, α (or Re), and, in the case of black-hole disks, the spin a.

2.3 Kinetic equilibrium and NLTE

● Kinetic equilibrium equations

Since one does not assume Local Thermodynamic Equilibrium (LTE), the atomic level populations have to be determined by solving the corresponding kinetic equilibrium equation. To this end, one selects the set of chemical species, each with a number of ionization stages, and for each stage a number of energy levels, for which the kinetic equilibrium equation is solved. These are called *explicit atoms*, *explicit ions*, and *explicit levels*, respectively. Their choice is completely driven by input data, described in Paper III, Chaps. 3, 4, and 11.

For each explicit atomic species, I, the set of kinetic equilibrium equations may be written as

$$\boldsymbol{\mathcal{A}_I \cdot n_I = b_I,} \tag{61}$$

where $\mathcal{A}$ is the rate matrix, $\mathbf{n} \equiv \{n_1, n_2, \ldots, n_{NL_I}\}$ is a vector of populations (number densities) of all explicit levels (in all ionization stages); their number being NL_I. In the following, we will drop subscript I.

We stress that the term "level" means here either a genuine energy eigenstate of an atom/ion, or several states lumped together (for instance a level composed of all components of a multiplet), or even the so-called *superlevel*, which is an aggregate of many different energy levels; for details, see § 3.6.

The elements of the rate matrix $\mathcal{A}$ are given by

$$\mathcal{A}_{ii} \quad = \quad \sum_{j \neq i}(R_{ij} + C_{ij}), \tag{62}$$

$$
\begin{align}
\mathcal{A}_{ij} &= -(R_{ji} + C_{ji}), \quad \text{for } j \neq i \text{ and } i \neq k, \tag{63} \\
\mathcal{A}_{kj} &= 1, \qquad\qquad \text{for } j = 1, \ldots, NL_I, \tag{64}
\end{align}
$$

where R_{ij} and C_{ij} are the radiative and collisional rates, respectively, and k is the index of the *characteristic level*, i.e. the level for which the rate equation is replaced by the particle conservation (abundance definition) equation.

Assuming $i < j$, the radiative rates are given by

$$
R_{ij} = \frac{4\pi}{h} \int_0^\infty \frac{\sigma_{ij}(\nu)}{\nu} J_\nu d\nu, \tag{65}
$$

$$
R_{ji} = \frac{4\pi}{h} \int_0^\infty \frac{\sigma_{ij}(\nu)}{\nu} G_{ij}(\nu) \left(\frac{2h\nu^3}{c^2} + J_\nu \right) d\nu, \tag{66}
$$

where $\sigma_{ij}(\nu)$ is the corresponding cross section, and $G_{ij}(\nu)$ is defined by

$$
G_{ij}(\nu) \equiv \begin{cases} g_i/g_j, & \text{for bound–bound,} \\ n_{\mathrm{e}}\Phi_i(T) \exp(-h\nu/kT), & \text{for bound–free.} \end{cases} \tag{67}
$$

where g_i is the statistical weight, n_{e} the electron density, and $\Phi_i(T)$ is the Saha-Boltzmann factor,

$$
\Phi_i(T) = \frac{g_i}{2g_1^+} \left(\frac{h^2}{2\pi m_{\mathrm{e}}kT} \right)^{3/2} e^{(E_I - E_i)/kT}; \tag{68}
$$

E_I is the ionization potential of the ion to which level i belongs; E_i is the excitation energy of level i, g_1^+ is the statistical weight of the ground state of the next ion, and m_{e} the electron mass.

If one adopts an occupation probability formalism that describes bound level dissolution resulting from perturbations with neighboring particles (see §2.6) the above equation remains the same, replacing $\sigma_{ij}(\nu) \to \sigma_{ij}(\nu)w_j$, and

$$
G_{ij}(\nu) = \begin{cases} (g_i w_i)/(g_j w_j), & \text{for bound–bound,} \\ (w_i/w_j)n_{\mathrm{e}}\Phi_i(T) \exp(-h\nu/kT), & \text{for bound–free.} \end{cases} \tag{69}
$$

where w_i is the occupation probability of level i.

In many instances one employs the concept of *detailed radiative balance*. It is defined such as the transition $i \leftrightarrow j$ is in detailed radiative balance if $n_i R_{ij} = n_j R_{ji}$. This is numerically equivalent to setting $R_{ij} = R_{ji} = 0$. This concept is often used to compute intermediate NLTE models because they are usually easier to converge than the full NLTE models.

The collisional rates, assuming that only collisions with free electrons are important (again, $i < j$), are given by

$$
\begin{align}
C_{ij} &= n_{\mathrm{e}}\Omega_{ij}, \\
C_{ji} &= (n_i^*/n_j^*)C_{ij}, \tag{70}
\end{align}
$$

where Ω_{ij} is the collisional cross section, and n_i^* the LTE population of level i.

The complete set of kinetic equilibrium equations is written as

$$\mathcal{A} \cdot \mathbf{n} = \mathbf{b}, \tag{71}$$

where the full rate matrix $\mathcal{A}$ is a block–diagonal matrix composed of all the individual matrices $\mathcal{A}_I$, and in a similar manner for the vector of populations $\mathbf{n}$ and the right–hand–side vector $\mathbf{b}$ – see below.

In LTE, the kinetic equilibrium equation in the form of Eq. (71) is not solved. Instead, the atomic level populations are determined by the Saha-Boltzmann relation,

$$n_i^* = n_e n_1^+ \Phi_i(T), \tag{72}$$

where n_1^+ is the population of the ground state of the next higher ion. It is often instructive to introduce the NLTE *departure coefficient*, or a *b*-factor, as

$$b_i \equiv n_i/n_i^*, \tag{73}$$

that shows a magnitude of NLTE effects for a given level.

● Particle conservation equation

The set of rate equations for all levels of an atom would form a linearly dependent system. Therefore, one equation of the set has to be replaced by the *number conservation*; also called the *abundance definition equation*,

$$\sum_{i=1}^{NL_I} n_i(1 + S_i) = N_I \equiv A_I N_H = (N - n_e)\alpha_I, \tag{74}$$

where $A_I \equiv N_I/N_H$ is the *abundance* of the species I, defined here as a ratio of the total number of atoms I, in all degrees of ionization, to the total number of hydrogen atoms, per unit volume. The last equality introduces the notion of *fractional abundance*, $\alpha_I = A_I \big/ \sum_J A_J$ of the chemical element I. The summation extends over all species, including hydrogen (for which, by definition, $A_H = 1$). TLUSTY usually works in terms of chemical abundances with respect to hydrogen, but it also allows to define an abundance with respect to any other species, called *reference species*, to be able to compute models of extremely hydrogen–poor or even hydrogen–free atmospheres.

The set of abundances of the individual species forms another basic input parameter of the problem.

The factor S_i accounts for the (LTE) populations of the higher, non-explicit levels, and is given by

$$S_i = \begin{cases} 0 & \text{if } i \text{ is not the ground state an ion,} \\ n_e \Sigma_J & \text{if } i \text{ is the ground state of ion } J+1. \end{cases} \tag{75}$$

where Σ_J is the so-called upper sum for an ion J which expresses the total population of higher, non-explicit states of ion J. In the previous versions of

TLUSTY it was expressed through its partition function as (Hubeny 1988)

$$\Sigma_J = (h^2/2\pi m_\mathrm{e} kT)^{3/2} e^{\chi_J/kT}(U_J/g_1^{J+1}) - \sum_{i=1}^{NL_J} w_i \Phi_i(T), \qquad (76)$$

where the first term represents the total population of ion J, and the second term the LTE population of all explicit levels. Here χ_J the ionization energy of ion J, and U_J its partition function. However, an evaluation of the upper sum using Eq. (76) may sometimes be inaccurate. Moreover, when one uses a model atom with many explicit levels, the contribution of the upper levels is very small. Therefore, a safe and still reasonably accurate approach for models with a sufficient number of explicit levels is to set the upper sum to zero,

$$\Sigma_J = 0. \qquad (77)$$

This is actually used in TLUSTY, version 205, by default for all ions except neutral hydrogen and hydrogenic ions.

An accurate way of expressing the contribution of upper states is by introducing the so-called *merged level*. This approach is currently used only for hydrogen and hydrogenic ions. A merged level is a sort of superlevel (see § 3.6) representing all levels higher than the highest explicit regular level. Its population is given by the sum of LTE populations of these states, computed with the occupation probability (see § 2.6).

$$n_\mathrm{mer} = \sum_{j=NL+1}^{N^*} n_j^* = \sum_{j=NL+1}^{N^*} n_\mathrm{e} n_1^+ w_j \Phi_j(T), \qquad (78)$$

where n_1^+ is the population of the ground state of the next ion, which in the case of hydrogen is the proton number density, $n_1^+ = n_\mathrm{p}$. N^* is a large number, taken in TLUSTY as 80, but its exact value does not matter because the occupation probability for such high states is essentially zero.

A merged level is treated as an explicit level with statistical weight $g_\mathrm{mer} = \sum_{j=NL+1}^{N^*} w_j g_j \exp(E_j/kT)$, so that its Saha-Boltzmann factor is simply given by $\Phi_\mathrm{mer}(T) = CT^{-3/2} g_\mathrm{mer}/(2g_1^+)$, with $C = (h^2/2\pi m_\mathrm{e} k)^{3/2}$. Its energy is formally set to the ionization energy, $E_\mathrm{mer} = E_\mathrm{ion}$, and its occupation probability $w_\mathrm{mer} = 1$ because the occupation probabilities of the individual components are already included in g_mer. For a treatment of transitions involving the merged level, see § 2.5. If the merged level is set for an atom/ion I, then the upper sum has to be set to zero, $\Sigma_I = 0$, and all the level parameters are computed analytically.

The choice of the characteristic level, denoted k, is arbitrary. Usually, one either choses the last level ($k = NL_I$), or a level with the highest population. The elements of the right-hand-side vector $\mathbf{b}$ are given by

$$b_i = (N - n_\mathrm{e})\alpha_I \,\delta_{ki}, \qquad (79)$$

that is, the only non-zero element of **b** is the term corresponding to level k.

● Charge conservation equation

The condition of global charge neutrality is expressed as

$$\sum_i n_i Z_i + Q - n_e = 0, \tag{80}$$

where Z_i is the charge associated with level i; that is, $Z_i = 0$ for levels of neutral atoms, $Z_i = 1$ for levels for once ionized ions, etc., The summation in Eq. (80) extends over all levels of all ions of all species. Quantity Q accounts for the additional charge coming from the ions that are not treated explicitly – see § 2.7.

● Mass density, and fictitious massive particle density equations

The mass density is expressed in terms of atomic level populations as

$$\rho = \sum_i m_i n_i, \tag{81}$$

where m_i is the mass of the atom to which level i belongs. It can also be expressed as

$$\rho = (N - n_e)\,\mu m_H, \tag{82}$$

where m_H is the mass of the hydrogen atom, and μ the *mean molecular weight*, defined by

$$\mu = \sum_I \alpha_I (m_I/m_H) = \frac{\sum_I A_I (m_I/m_H)}{\sum_I A_I} \tag{83}$$

where m_I is the mass of an atom of species I.

One can also introduce a *fictitious massive particle density*, defined as

$$n_m \equiv (N - n_e)\mu, \tag{84}$$

so that the mass density can be written as

$$\rho = n_m m_H. \tag{85}$$

This option is offered in TLUSTY, but is rarely used.

2.4 Absorption, emission, and scattering coefficients

● Absorption

The above set of structural equations has to be complemented by equations defining the absorption and emission coefficients.

The absorption coefficient (or opacity) is given by

$$\chi_\nu = \kappa_\nu + \kappa_\nu^{sc}, \tag{86}$$

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where κ_ν is the extinction coefficient (sometimes called the true absorption coefficient), and κ_ν^{sc} is the scattering coefficient. The extinction coefficient is given by

$$
\begin{aligned}
\kappa_\nu \;=\;& \sum_i \sum_{j>i} \left[n_i - n_j G_{ij}(\nu) \right] \sigma_{ij}(\nu) + \sum_i \left[n_i - n_k G_{ik}(\nu) e^{-h\nu/kT} \right] \sigma_{ij}(\nu) \\
& + \sum_\kappa n_{\mathrm{e}} n_\kappa \sigma_{\kappa\kappa}(\nu,T) \left(1 - e^{-h\nu/kT} \right) + \kappa_\nu^{\mathrm{add}},
\end{aligned}
\tag{87}
$$

where the first term represents the contribution of the bound–bound transitions, the second term the bound–free transitions (with k being the final state of the corresponding process), and the third term the free–free transitions. The summations extends over all level of all species. The term $\kappa_\nu^{\mathrm{add}}$ represents any additional opacity. It is used to account for opacity sources that are not written in terms of explicit bound–bound or bound–free transitions.

The scattering part of the absorption coefficient is given by

$$
\kappa_\nu^{\mathrm{sc}} = n_{\mathrm{e}} \sigma_{\mathrm{e}} + \sum_i n_i \sigma_{\mathrm{Ray},i}
\tag{88}
$$

where the first term accounts for electron scattering, and the second term for the Rayleigh scattering. Here σ_{e} is the Thomson cross section, $\sigma_{\mathrm{Ray},i}$ is the Rayleigh scattering cross section of species i, and n_i is the number density of species i. The summation extends over all species for which Rayleigh scattering gives a non–negligible contribution to the total scattering opacity.

For high-energy objects (extremely hot white dwarfs or hot accretion disks), one may consider an inelastic electron scattering, called Compton scattering, as described in Hubeny et al. (2001). A brief outline is given below, and for more details refer to Paper III, § 12.5.

● Emission

The total emission coefficient is also given as a sum of thermal and scattering contributions. The latter refers only to *continuum scattering*; scattering in spectral lines is usually treated with complete frequency redistribution, in which case the scattering is in fact a part of the thermal emission coefficient. The continuum scattering part is usually treated separately from the thermal part, and the "thermal emission coefficient" is usually called the "emission coefficient." Specifically,

$$
\eta_\nu^{\mathrm{tot}} = \eta_\nu + \eta_\nu^{\mathrm{sc}},
\tag{89}
$$

where

$$
\begin{aligned}
\eta_\nu \;=\;& (2h\nu^3/c^2) \Bigg[\sum_j \sum_{j>i} n_j G_{ij}(\nu) \sigma_{ij}(\nu) + \sum_i n_k G_{ik}(\nu) \sigma_{ik}(\nu) e^{-h\nu/kT} \\
& + \sum_\kappa n_{\mathrm{e}} n_\kappa \sigma_{\kappa\kappa}(\nu,T) e^{-h\nu/kT} \Bigg] + \eta_\nu^{\mathrm{add}}.
\end{aligned}
\tag{90}
$$

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The additional emissivity, if included, is usually given by $\eta_\nu^{\mathrm{add}} = \kappa_\nu^{\mathrm{add}} B_\nu$; with B_ν being the Planck function. The form of the scattering part of the emission coefficient depends on additional assumptions – see below. In the simple case that we assume an isotropic phase function, and electron scattering is treated as coherent Thomson scattering, then

$$\eta_\nu^{\mathrm{sc}} = \kappa_\nu^{\mathrm{sc}} J_\nu. \tag{91}$$

• Scattering

Various scattering mechanisms are treated differently, depending on their nature. The three types of scattering TLUSTY is designed to treat are the following:

– *Thomson and Rayleigh scattering.* These scattering processes are coherent (without a change in frequency of the absorbed and scattered photon), and they are also approximated to be isotropic. Consequently, their treatment is simple. As follows from equations (88) and (91), the total source function is given by

$$S_\nu^{\mathrm{tot}} = \frac{\eta_\nu}{\chi_\nu} + \frac{\kappa_\nu^{\mathrm{sc}}}{\chi_\nu} J_\nu, \tag{92}$$

so that the scattering part of the source function, the second term in equation (92), is simply proportional to the mean intensity at the same frequency, which does not cause any numerical complications.

– *Scattering in spectral lines*, If one assumes complete frequency redistribution in all lines, as is done in equation (90), the emission coefficient for lines does not contain the radiation intensity explicitly (it enters implicitly through the solution of kinetic equilibrium equation that contains radiative rates), so that formally there is no distinction between the thermal and scattering processes in a line.

TLUSTY also offers an approximate treatment of partial frequency redistribution, through the so-called partial coherent scattering approximation; for a detailed discussion, refer to Hubeny & Mihalas (2014; § 15.3). This option is rarely used, and is briefly described in § 12.9.1.

– *Compton scattering* is a non-coherent electron scattering, which is particularly important for high temperature models at high photon energies.. It is important for hot accretion disks (Seyfert galaxies, X-ray binary disks), and also for extremely hot white dwarfs, possibly with a hydrogen-burning layer on their surface (the so-called super-soft sources), or pre-white dwarfs. Its treatment in TLUSTY follows from the formalism of Hubeny et al. (2001), which is based on a Kompaneets approximation (e.g., Rybicki & Lightman, 1979), for which the Compton scattering part of the source function is given by

$$S_\nu^{\mathrm{Compt}} = (1-x)J_\nu + (x - 3\Theta)J_\nu' + \Theta J_\nu'' + \frac{c^2}{2h\nu^3} J_\nu 2x(J_\nu' - J_\nu), \tag{93}$$

where

$$x = \frac{h\nu}{m_{\mathrm{e}}c^2}, \quad \Theta = \frac{kT}{m_{\mathrm{e}}c^2}, \tag{94}$$

and

$$J'_\nu \equiv \frac{\partial J_\nu}{\partial \ln \nu}, \quad J''_\nu \equiv \frac{\partial^2 J_\nu}{\partial (\ln \nu)^2}. \tag{95}$$

A discretization of equations (93) and (95) and their implementation in the linearization scheme, is described in detail in Hubeny et al. (2001; Appendix A); see also Paper III, § 12.5.

2.5 Atomic transition processes

A treatment of atomic transitions, in particular the corresponding cross sections, is an important ingredient of the modeling process, for both stellar atmospheres and accretion disks. Although handling of transition cross sections is essentially transparent for a casual user because most of the atomic data is communicated to the code through the set of already prepared atomic data files (see Paper III, Chap. 11), there is still a possibility for the user to choose from several options, or add specific processes that operate on, or are important only for certain classes of objects. This is done by specific keyword parameters, that are be described in Paper III, Chap. 12.

The two essential classes of transitions are the *radiative* (an interaction of an atom/ion with a photon) and the *collisional* (an interaction of an atom with another particle, typically electron) transitions. We will briefly describe them in the following.

2.5.1 Bound-bound radiative transitions

TLUSTY distinguishes two types of bound-bound processes (lines):
– ordinary line – a transition between two ordinary levels;
– superline – a transition involving a superlevel, i.e. a transition between an ordinary level and superlevel, or between two superlevels.

● Ordinary lines

The cross section for an ordinary line that enters equations (65) and (66) for radiative rates, as well as equations (87) and (90) for the opacity and emissivity, is given by

$$\sigma_{ij}(\nu) = \frac{\pi e^2}{m_e c} f_{ij} \phi_{ij}(\nu), \tag{96}$$

where f_{ij} is the oscillator strength, and $\phi_{ij}(\nu)$ is the normalized absorption profile coefficient. There are several possibilities to adopt for the profile coefficient:

(i) *Doppler profile*,

$$\phi(\nu) = \frac{1}{\sqrt{\pi}\Delta\nu_D} \exp(-x^2), \tag{97}$$

where $x = (\nu - \nu_{ij})/\Delta\nu_D$ is the frequency displacement from the line center, ν_{ij}, expressed in units of the Doppler width, $\Delta\nu_D$. The latter is given by

$$\Delta\nu_D = \frac{\nu_{ij}}{c} \sqrt{\frac{2kT}{m_A} + v_{\text{turb}}^2}, \tag{98}$$

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where m_A is the mass of the atom, and v_{turb} is the turbulent velocity. The profile depends on temperature, and therefore depends on depth and changes from iteration to iteration. Experience revealed (e.g., Werner 1987) that one can safely use a simplified approach in which a characteristic temperature is chosen [typically $T = (3/4)T_{\text{eff}}$] with which the line profile is computed at the beginning and is stored for further use during the whole iteration process. This option is offered in TLUSTY, and is often being used, although considering depth-dependent Doppler profile does not lead to any significant additional time consumption. There is an additional subtle point. The frequency points for a line are chosen to provide accurate values of the integrals over frequency. Their setting is also based on using a characteristic temperature. When a modest number of frequency points is considered, using depth-independent Doppler profile assures that the evaluation of radiative rates and other integrals over frequency is accurate at all depth points, which is not necessarily true if a depth-dependent profile is assumed. In order to treat a depth-dependent profile accurately at all depth points, one would need to select many more frequency points.

(ii) *Voigt profile*,

$$\phi(\nu) = \frac{1}{\sqrt{\pi}\Delta\nu_D} H(a, x), \tag{99}$$

where H is the Voigt function, and a is the damping parameter expressed in units of Doppler width, $a = \Gamma/(4\pi\Delta\nu_D)$. The damping parameter is usually composed of three parts, corresponding to natural (lifetime) broadening, Stark broadening, and Van der Waals broadening.

(iii) *Special hydrogen line profiles.* For the purposes of model construction it is possible to consider hydrogen lines with a Doppler profile, as was done in the past, see e.g. Mihalas (1978). However, it is preferable to take the profile coefficients in a more accurate form. TLUSTY offers three possibilities, ordered here with increasing accuracy:
– a simple approximation by Hubeny, Hummer, & Lanz (1995; Appendix A), that essentially gives a Doppler profile in the line center, a Holtsmark profile in the wings, and a simple bridging law in the intermediate region.
– using tables computed by Lemke (1997) for the first members of the Lyman, Balmer, Paschen, and Brackett series up to the higher level with main quantum number $n = 10$ (the tables contain more lines, but the results for lines with $n > 10$ were found to be incorrect);
– using Tremblay-Bergeron (2009) tables, that take into account the effects of level dissolution, and are therefore the most accurate ones, in particular for high densities, and so preferable for instance for white dwarf models.

To describe an ordinary line, one therefore needs the *oscillator strength* (or, equivalently, one of the Einstein coefficients), the line center frequency (which is given by the difference of level energies), a switch indicating the choice of the type of profile, and in case of a Voigt profile, parameters that specify the damping parameters. All these parameters are communicated to the code through the corresponding entries in the input atomic data files – see Paper III, § 11.3

and § 12.1.1.

- Superlines

    The cross sections for superlines can be treated in two different ways:
    – using the Opacity Distribution Functions (ODF); or
    – using the Opacity Sampling (OS) approach.

    The ODF approach, which consists of resampling a complicated composite cross section for a superline to form a monotonic function of frequency, was used in the past (e.g., Hubeny & Lanz 1995), and although it is still offered by TLUSTY, it is outdated, and will not be described here.

    The OS approach is the standard one used in TLUSTY to describe a superline cross section. It is evaluated by summing the contributions from the individual ordinary lines that form the superline. The name Opacity Sampling comes from the fact that one computes the composite cross section for a set of frequency points that are in principle randomly distributed, and do not necessarily have to describe all the details of the exact cross section. In other words, the composite cross section may miss cores of some lines, and may miss some windows between lines, but in a statistical sense provides a reasonable description. The frequency sampling used in TLUSTY is simply a set of equidistantly spaced frequencies with a frequency step that is set up by input data. When decreasing the sampling step, one in fact recovers an essentially exact form of the composite cross section. This is the approach used for instance in the computed grids of NLTE metal line-blanketed model atmospheres for O and B stars (Lanz & Hubeny 2003, 2007).

2.5.2 Bound-free radiative transitions

Bound-free (photoionization) cross sections for transitions from ordinary levels are evaluated using various standard formulae. For hydrogen and hydrogenic ions one uses the standard hydrogenic cross section (e.g., Hubeny & Mihalas 2014, eq. 7.91), viz.

$$\sigma_{\rm bf}(\nu) = \frac{64\pi^4 Z^4 e^{10} m_{\rm e}}{3\sqrt{3}ch^6} \frac{\bar{g}_{\rm bf}(n,\nu)}{n^5\nu^3} = 2.815 \times 10^{29}\, Z^4\, \frac{\bar{g}_{\rm bf}(n,\nu)}{n^5\nu^3}, \qquad (100)$$

where n is the main quantum number of the lower bound state, Z is the charge of the ion ($Z = 1$ for hydrogen), and $\bar{g}_{\rm bf}(n,\nu)$ is the bound-free Gaunt factor. By default, it is evaluated by an analytical approximation as in Mihalas et al.(1975), but TLUSTY offers some alternative expressions. For details, refer to Paper III, § 11.2.

For other species, the cross sections may be evaluated by various approximate fitting formulae (which is an outdated option, although still available in TLUSTY), or, for most transitions, by tabular values based on the Opacity Project (OP – Seaton 1995) calculations. They are described in detail in Paper III, § 11.2. The values are already included in the atomic data files, so that the user does not have to provide any additional information, unless they want

to change or improve the default cross sections. For levels for which no cross sections are available, hydrogenic form is usually assumed.

The OP cross sections contain a number of photoionization resonances. Before transporting them to the TLUSTY input atomic data files, they are usually smoothed, forming the so-called *resonance-averaged profile* (RAP), see, e.g., Allende Prieto et al. (2003). The smoothing serves two purposes. Firstly, it decreases the number of frequency points needed to represent the cross section. However, since the number of frequencies is large anyway, this is not critical. Secondly, and more importantly, it avoids spurious peaks in the cross sections that may arise due to an insufficient frequency resolution adopted in the original atomic structure calculations. The cross sections are then represented by several tens up to several hundred values. For details, refer to Paper III, § 7.7.

For bound-free transitions from superlevels, the photoionization cross sections are pre-calculated by summing the cross sections of the individual components, and stored in special input files – see Paper III, § 11.2.

The inverse process, the radiative recombination, is described by the same cross section as for the photoionization. Because the cross sections include resonances, there is no need to consider the dielectric recombination as a separate process, or requiring separate data for dielectronic recombination rate (although such on option is also included in TLUSTY for historical reasons). For a discussion of the physics, see Hubeny & Mihalas (2014, § 9.3), and for details on the numerical implementation in TLUSTY, see Paper III, § 12.3.3.

2.5.3 Inner-shell photoionization

In order to better describe high temperature structures where the X-ray flux is dominant, a simple treatment of the inner-shell photoionization, or Auger process, has been implemented in TLUSTY by Hubeny et al. (2001). It employs a simplifying assumption that if an Auger electron is energetically possible, than it is in fact produced and the photoionization results in a jump by two stages of ionization to a ground state configuration. Therefore, both fluorescence and multiple Auger electron ejection arising from inner shell photoionization are neglected. The necessary data were taken from the X-ray photoionization code XSTAR (Kallman 2000)

In practice, a different structure of input atomic data is employed for ions for which one allows inner-shell photoionization processes. They are described in more detail in Paper III, § 11.7.

2.5.4 Free-free radiative transitions

The cross section is given by the standard formulae [e.g. Hubeny & Mihalas (2014, eq. 7.100)]

$$\sigma_{ff}(\nu, T) = \frac{\sqrt{32\pi} Z^2 e^6 \bar{g}_{ff}(\nu, T)}{3\sqrt{3} ch (km_e^3)^{1/2}} \frac{1}{T^{1/2}\nu^3} = 3.69 \times 10^8 Z^2 \bar{g}_{ff}(\nu, T) \frac{1}{T^{1/2}\nu^3}, \quad (101)$$

where $\bar{g}_{ff}(\nu, T)$ is the free-free Gaunt factor. It is evaluated by the approximate expression as in Mihalas et al. (1975). For non-hydrogenic ions, one still uses formula (101) with the Gaunt factor set to unity, $\bar{g}_{ff}(\nu, T) = 1$. In the past, one usually employed a *modified free-free* cross section (Mihalas et al. 1975) that contained a contribution of photoionization from higher, non-explicit levels taken in a hydrogen approximation (since all these have a common ν^{-3} frequency dependence). This option is still being offered in TLUSTY, but is essentially obsolete. It is briefly described in Paper III, §4.32.

2.5.5 Particle-induced transitions (collisions)

• Collisions with electrons

By default, one considers collisions with electrons, for both bound-bound and bound-free transitions. The code contains a number of hardwired expressions for evaluating the electron collision rates. The user can either employ a default expression, or choose some other form of expression. For details, refer to Paper III, §11.2 and §11.3.

• Charge transfer reactions

TLUSTY offers an option to include one such particular reaction, namely the single electron exchange with neutral hydrogen,

$$X^Z + H \leftrightarrow X^{Z-1} + H^+, \tag{102}$$

in which species X in ionization stage Z exchanges an electron with hydrogen, becoming an ion with charge $Z - 1$ (charge-exchange recombination), or an inverse process (charge-exchange ionization). The reaction rates are taken from Kingdon & Ferland (1996) who provide useful analytical fits to theoretical as well as experimental results in the form

$$\sigma_{\rm rec}(T) = a T_4^b (1 + e^{dT_4}), \tag{103}$$

with $T_4 = T/10^4$, and a, b, d being the fitting parameters. For more details, refer to Paper III, §12.3.2.

2.6 Level dissolution; occupation probabilities, and pseudocontinua

An improved description of the atomic level populations and related transition rates, also implemented in TLUSTY, adopts the concept of occupation probabilities and level dissolution (Hummer & Mihalas 1988; Hubeny, Hummer & Lanz 1994; Hubeny & Mihalas 2014, § 9.4). It is based on introducing the *occupation probability* of a level. In LTE, it is given through the generalized Boltzmann formula,

$$(n_i/n_I)^* = w_i(g_i/U_I)e^{-E_i/kT}, \tag{104}$$

where the occupation probability w_i is the probability that an atom is in state i relative to that in a similar ensemble of non-interacting atoms. The same

general definition applies also in the case of NLTE. Correspondingly, $(1 - w_i)$ is the probability that the state i is dissolved, i.e., it lies in the continuum, or, in other words, the corresponding electron instead of being in the bound state j is in fact free.

The transition from a lower bound state i to the state j is therefore split into two parts: (i) a transition to a non-dissolved fraction of the level forms an ordinary line, while (ii) a transition to the dissolved fraction of the level is in fact a bound-free process, called *pseudocontinuum*. The total pseudocontinuum cross section is a sum of the contributions from the dissolved fractions of all the states j higher than i. It is very difficult to compute it exactly; the current expression is based on the approximation devised by Daeppen et al. (1987) and Hubeny, Hummer, & Lanz (1994), viz.

$$\sigma_{ik}^{\text{tot}}(\nu) = D_i(\nu)\sigma_{ik}^{\text{ext}}(\nu), \tag{105}$$

where $\sigma_{ik}^{\text{ext}}(\nu) = \sigma_{ik}(\nu)$ for $\nu \geq \nu_{ik}$ is a usual cross section for the bound-free transition from level i, while for $\nu < \nu_{ik}(\nu)$ represents an extrapolated cross section; ν_{ik} is the ionization frequency from level i, and D_i is the so-called dissolved fraction, approximated by

$$D_i(\nu) = \begin{cases} 1 & \text{if} \quad \nu \geq \nu_{ik}, \\ 1 - w_{m_{i*}}(\nu) & \text{if} \quad \nu < \nu_{ik}. \end{cases} \tag{106}$$

where $m_{i*}(\nu) = [i^{-2} - (\nu/\nu_{ik})]^{-1/2}$ is an effective quantum number of the highest state that can be reached from state i by the absorption of a photon with frequency ν. It does not have to be an integer. Its occupation probability is computed by the same analytic expression as for integer values, Eqs. (107) - (108).

Equation (105) was derived, and is reasonably accurate, for frequencies close to the ionization threshold. Since for decreasing frequency $w_{m_{i*}} \to 1$ as $m_{i*} \to 1$, it was originally believed that Eq. (106) can be used even far from the threshold, but it turned out that its contribution can be numerically non-negligible or even in some cases dominant very far from the threshold where its application is completely unphysical. Therefore, we have to introduce an empirical cutoff, so equation (105) is applied only for $\nu > \nu^{\text{cutoff}}$. This quantity is a parameter in TLUSTY transported through the atomic data file. Typically it is taken as $\nu^{\text{cutoff}} \approx 3 \times 10^{15}$ for the Lyman pseudocontinuum, and $\nu^{\text{cutoff}} \approx 7 \times 10^{14}$ for the Balmer pseudocontinuum.

After Hubeny, Hummer, & Lanz (1994), the occupation probability is given by

$$w_i = f/(1 + f), \quad \text{with} \quad f = \frac{0.1402(x + 4Z_r a^3)\beta_c^3}{1 + 0.1285x\beta_c^{3/2}}, \tag{107}$$

where $a = 0.09 \times n_e^{1/6}T^{-1/2}$, $x = (1 + a)^{3.15}$ and Z_r is the radiator charge, and the critical field strength β_c is given by

$$\beta_c = 8.59 \times 10^{14} Z^3 n_e^{-2/3} k_i i^{-4}, \tag{108}$$

where $k_i = 1$ for $i \leq 3$, and $k_i = (16/3)i/(i+1)^{-2}$ for $i > 3$.

When this formalism [based on an earlier version of the theory directly from Hummer & Mihalas (1988)] was applied in actual models, it was found (Bergeron, Wesemael, & Fontaine 1991) that the agreement between predicted and observed hydrogen line profiles of white dwarfs was significantly improved if the critical field strength β_c is multiplied by an empirical factor of 2. This correction was originally applied in TLUSTY as well; however, later it tuned out that the Bergeron correction was relevant only to the original Hummer-Mihalas expressions for occupation probabilities. When using an improved version (first presented in Hubeny, Hummer, & Lanz 1994; Appendix A), such a correction is unnecessary or even incorrect. This option is still included in TLUSTY for testing purposes, but should not be used for actual models.

Eqs. (107) - (108) apply for perturbations by charged particles. For cooler models one should also include occupation probabilities due to perturbations with neutral perturbers. This is not yet implemented in the current version of TLUSTY.

2.7   Equation of state and molecules

2.7.1   Atoms and ions only

In the original implementation of TLUSTY, the equation of state was not formulated explicitly; it has only been used as a relation between the gas pressure P and the total particle number density, N – see equation (13). At the same time, the mass density is given by equation (82). The total particle number density is given by the sum of all level populations of all individual explicit species in all explicit ionization stages. However, such a simple definition would miss the contribution of species that are not treated explicitly. To include them, one selects a set of implicit species, which are usually all the remaining species that are not treated explicitly (but their choice may be set differently by input data). Their ionization balance is treated in LTE, that is, it is assumed to obey the Saha equation,

$$(N_{I,J}/N_{I+1,J}) = n_{\mathrm{e}} \left(U_{I,J}/U_{I+1,J}\right) \left(h^2/2\pi m_{\mathrm{e}}kT\right)^{3/2} e^{\chi_{I,J}/kT}, \qquad (109)$$

supplemented by the condition for the total abundance of the element,

$$\sum_I N_{I,J} = N_J = (N - n_{\mathrm{e}})\alpha_J = (N - n_{\mathrm{e}})A_J \Big/ \sum_{J'} A_{J'}, \qquad (110)$$

where J is the index of the atom to which the ions I belong, A_J is the abundance of species J with respect to hydrogen, $A_J \equiv N_J/N_H$, and α_J is the fractional abundance. The additional charge Q in Eq. (80) is given by

$$Q = \sum_J \sum_I N_{I,J} Z_I, \qquad (111)$$

where Z_I is the charge of ion I.

The adopted chemical abundances may be set by the input data (see Paper III, §4.2), but if nothing is specified, the default abundances are given by the solar abundances. The adopted solar abundances of the first 30 elements (by number, with respect to hydrogen), essentially after Grevesse & Sauval (1998), are listed in Table 2.

2.7.2 Standard evaluation of the partition functions

Let A be the atomic number, and Z the charge of the ion ($Z = 0$ for neutrals). The following references are used for the individual groups of species. In some cases, there is a choice of several source, driven by additional input – see Paper III, §12.7.

- for $A \leq 30$ and $Z \leq 4$, unless specified otherwise (see Paper III, §12.7), an evaluation after Traving, Baschek, & Holweger (1966);

- for $A \leq 30$ and $Z \leq 2$, and for the local temperature $T \leq 16,000$ K, the default partition function is evaluated after Irwin (1980);

- for $A > 30$ and $Z \leq 2$, after Kurucz (1970);

- for $A = 26$ (Fe) or $A = 28$ (Ni), and $3 \leq Z \leq 8$, after Sparks & Fischel (1971);

- for $6 \leq A \leq 8$ (CNO) and $Z > 4$, after Sparks & Fischel (1971).

- for $A \leq 30$ (except C,N,O) and $Z > 4$, approximate partition function given by the statistical weight of the ground state;

2.7.3 Molecules

The situation is more complicated when the formation of molecules begins to contribute. In this case, one assumes that free atoms exist only in the neutral and once ionized states, and that there is a number of molecular species. In this case, we assume LTE. Their number densities are governed by a general Saha equation

$$N_{1,\ldots,m}^{+Z} \equiv N_{\{1,m\}}^{+Z} = \frac{\prod_{i=1}^{m} N_i}{n_{\mathrm{e}}^{Z}} \Phi \qquad (112)$$

where

$$\Phi = \frac{U_{\{1,m\}}^{+Z}(2\pi M_{\{1,m\}}kT/h^2)^{3/2} \left[2(2\pi m_{\mathrm{e}}kT/h^2)^{3/2}\right]^{Z}}{\prod_{i=1}^{m} U_i(2\pi M_i kT/h^2)^{3/2}} e^{-\Delta E/kT}, \qquad (113)$$

with

$$\Delta E = E_{\{1,m\}}^{+Z} - \sum_{i=1}^{m} E_i, \qquad (114)$$

where $X_{\{1,m\}}^{+Z}$, with $X \equiv N, U, M, E$, denotes a quantity associated with composite particle with charge Z composed of m atomic species $1, \ldots, m$; some

Table 2: Adopted solar abundances from Grevesse & Sauval (1998).

Element	$N_{\mathrm{el}}/N_{\mathrm{H}}$
H	1.0
He	1.00×10^{-1}
Li	1.26×10^{-11}
Be	2.51×10^{-11}
B	5.00×10^{-10}
C	3.31×10^{-4}
N	8.32×10^{-5}
O	6.76×10^{-4}
F	3.16×10^{-8}
Ne	1.20×10^{-4}
Na	2.14×10^{-6}
Mg	3.80×10^{-5}
Al	2.95×10^{-6}
Si	3.55×10^{-5}
P	2.82×10^{-7}
S	2.14×10^{-5}
Cl	3.16×10^{-7}
Ar	2.52×10^{-6}
K	1.32×10^{-7}
Ca	2.29×10^{-6}
Sc	1.48×10^{-9}
Ti	1.05×10^{-7}
V	1.00×10^{-8}
Cr	4.68×10^{-7}
Mn	2.45×10^{-7}
Fe	3.16×10^{-5}
Co	8.32×10^{-8}
Ni	1.78×10^{-6}
Cu	1.62×10^{-8}
Zn	3.98×10^{-8}

components may be identical. Here N, U, M, E stands for number density, partition function, mass, and energy, respectively. Here we consider only $Z = 0$ or $Z = 1$; and for negative ions of atoms or molecules, electrons are considered as a separate atomic species. The critical quantity of Φ is given either by its definition, Eq. (113), if all the partition functions are available, or is represented by a fitting formula, e.g., the one used by Kurucz (1970; eq. 4.35)

$$\Phi(T) = \exp\left[\frac{\Delta E}{kT} - b + cT - dT^2 + eT^3 - fT^4 - \frac{3}{2}(m - 1 - Z)\ln T\right], \quad (115)$$

where ΔE, b, c, d, e, and f are the fitting parameters. For some species one uses a different fitting formula by Tsuji (with data kindly supplied by Uffe Jorgenssen, priv. comm.).

Equation (112) is supplemented by the set of particle conservation equations for all considered chemical elements, A,

$$\sum_{k=1}^{NS} N_k^{+Z} c_k^A = N_A = (N - n_e)\alpha_A, \quad (116)$$

and the charge conservation equation

$$\sum_{k=1}^{NS} N_k^{+Z} Z c_k^A = n_e, \quad (117)$$

where NS is the total number of species, atomic or molecular, N_k is the number density of species k, where k numbers all composited species denoted with subscript $\{1, m\}$, and c_k^A is the number of atoms A in the species k (for instance, if species k is water H_2O, then $c_k^H = 2$, $c_k^O = 1$, and $c_k^X = 0$ for all other elements X).

3   Numerical procedure

The set of structural equations (1) with boundary conditions (5) and (9), (15), (16) or (19), (71), (80), and necessary auxiliary expressions, are discretized in depth and frequency, replacing derivatives by differences and integrals by quadrature sums. This yields a set of non-linear algebraic equations. Detailed forms of the discretized equations are summarized in Hubeny & Mihalas (2014; § 18.1).

Upon discretization, the physical state of an atmosphere is fully described by the set of vectors ψ_d for every depth point d, $(d = 1, \ldots, ND)$, ND being the total number of discretized depth points. The full state vector ψ_d is given by

$$\psi_d = \{J_1, \ldots, J_{NF}, N, T, n_e, n_1, \ldots, n_{NL}, [n_m], [\nabla], [z]\}, \quad (118)$$

where J_i is the mean intensity of radiation in the i-th frequency point; we have omitted the depth subscript d. The quantities in the square brackets are

optional, and are considered to be components of vector ψ only in specific cases: n_m if specifically selected; ∇ if convection is taken into account, and z in the case of disks. The dimension of the vector ψ_d is NN, $NN = NF + NL + NC$, where NF is the number of frequency points, NL the number of atomic energy levels for which the rate equations are solved (i.e., explicit levels), and NC is the number of constraint equations ($NC = 3$ in the standard atmospheric case, but it can be as large as 6).

3.1 Linearization

Although the individual methods of the solution differ, the resulting non-linear algebraic equations are solved by some kind of linearization. In the general case, the solution proceeds as a direct application of the Newton-Raphson method. Suppose the required solution ψ_d can be written in terms of the current, but imperfect, solution ψ_d^0 as $\psi_d = \psi_d^0 + \delta\psi_d$. The entire set of structural equations can be formally written as an operator P acting on the state vector ψ_d as

$$P_d(\psi_d) = 0. \tag{119}$$

To obtain the solution, we express $P_d(\psi_d^0 + \delta\psi_d) = 0$, and assuming that $\delta\psi_d$ is "small" compared to ψ_d we use a Taylor expansion of P:

$$P_d(\psi_d^0) + \sum_j \frac{\partial P_d}{\partial \psi_{d,j}} \delta\psi_{d,j} = 0. \tag{120}$$

to solve for $\delta\psi_d$. Because only a first–order (i.e., linear) term of the expansion is taken into account, this approach is called a *linearization*. To obtain the corrections $\delta\psi_d$, one has to form a matrix of partial derivatives of all the equations with respect to all the unknowns at all depths—the *Jacobi matrix*, or *Jacobian*—and to solve equation (120). The kinetic equilibrium and charge conservation equations are *local*, that is, for depth point d they contain the unknown quantities ψ_d only at depth d. The radiative equilibrium equation (in the differential form), and the hydrostatic equilibrium equation couple two neighboring depth points $d-1$ and d. The radiative transfer equations couple depth point d to two neighboring depths $d-1$ and $d+1$; see equations (1) – (8). Consequently, the system of linearized equations can be written as

$$-\mathbf{A}_d \delta\psi_{d-1} + \mathbf{B}_d \delta\psi_d - \mathbf{C}_d \delta\psi_{d+1} = \mathbf{L}_d, \tag{121}$$

where A, B, and C are $NN \times NN$ matrices, and L is a residual error vector, given by

$$\mathbf{L}_d = -P_d(\psi_d^0). \tag{122}$$

At the convergence limit, $L \to 0$ and thus $\delta\psi_d \to 0$.

Equation (121) is solved by a standard Gauss-Jordan elimination that consists of a forward elimination

$$\mathbf{D}_1 = \mathbf{B}_1^{-1}\mathbf{C}_1, \quad \text{and} \quad \mathbf{D}_d = (\mathbf{B}_d - \mathbf{A}_d\mathbf{D}_{d-1})^{-1}\mathbf{C}_d, \quad d = 2, \ldots, ND, \tag{123}$$

and

$$\mathbf{Z}_1 = \mathbf{B}_1^{-1}\mathbf{L}_1, \quad \text{and} \quad \mathbf{Z}_d = (\mathbf{B}_d - \mathbf{A}_d\mathbf{D}_{d-1})^{-1}(\mathbf{L}_d + \mathbf{A}_d\mathbf{Z}_{d-1}), \quad d = 2, \ldots, N. \tag{124}$$

followed by a back-substitution

$$\delta\psi_{ND} = \mathbf{Z}_{ND}, \quad \text{and} \quad \delta\psi_d = \mathbf{D}_d\delta\psi_{d+1} + \mathbf{Z}_d, \quad d = ND - 1, \ldots, 1. \tag{125}$$

This procedure, known as *complete linearization*, was developed in the seminal paper by Auer & Mihalas (1969). However, since the dimension of the state vector ψ, that is the total number of structural parameters NN can be extremely large; for instance, in modern metal line blanketed model atmospheres NF has to be taken few times 10^5, a direct application of the original complete linearization is not practical. Various possibilities to improve the performance of the method are discussed in detail in Hubeny & Mihalas (2014, §18.3). There are several variants of such improvements which are implemented in TLUSTY.

3.2   Hybrid CL/ALI method

The method, developed by Hubeny & Lanz (1995), combines the basic advantages of the complete linearization (CL) and the accelerated lambda iteration method (ALI). For a general description of ALI, refer to Hubeny & Mihalas (2014; Chap. 13). The hybrid CL/ALI scheme is essentially a linearization method, except that the mean intensity in some (most) frequency points is not treated as an independent state parameter; instead it is expressed as

$$J_{di} = \Lambda_{di}^*(\eta_{di}/\kappa_{di}) + \Delta J_{di}, \tag{126}$$

where d and i represent indices of the discretized depth and frequency points, respectively, Λ^* is the so-called approximate Lambda operator, and ΔJ is a correction to the mean intensity. The approximate operator, in most cases taken as diagonal (local), so that its action is just an algebraic multiplication, is evaluated in the formal solution of the transfer equation, and is held fixed in the next iteration of the linearization procedure, and so is the correction ΔJ. Since the absorption and emission coefficients κ and η are known functions of temperature, electron density, and atomic level populations, one may express the linearization correction to mean intensity J_{di} as

$$\delta J_{di} = \sum_x \Lambda_{di}^* \frac{\partial(\eta_{di}/\kappa_{di})}{\partial x_{di}}\delta x_{di}, \tag{127}$$

where $x = (T, n_e, n_i)$, i.e., x stands for other state parameters –temperature, electron density, and level populations.

Equation (127) shows that J_{di} is effectively eliminated, thus reducing the size of vector ψ to $NN = NF_{CL} + NL + NC$, where NF_{CL} is the number of frequency points for which the mean intensity is kept to be linearized, called explicit frequencies. As shown in Hubeny & Lanz (1995), such a number can be

very small, of the order of $O(10^0)$ to a few times 10^1. Typically, only frequencies in the centers of the strongest lines, and a few frequencies just shortward of the edges of the strongest continua, are kept to be linearized.

The choice of which frequencies are linearized is driven by input data. TLUSTY can thus cover the whole range of options, from the pure complete linearization (no frequencies treated with ALI), to full ALI, in which no frequency points are linearized.

3.3 Rybicki scheme

An alternative scheme, which can be used in conjunction with either original complete linearization, or a hybrid CL/ALI scheme, is a generalization of the method developed originally by Rybicki (1969) for solving a line transfer problem. It starts with the same set of linearized state equations, and consists in a reorganization of the state vector and resulting Jacobi matrix in a different form. Instead of forming a vector of all state parameters in a given depth point, it constructs a set of vectors of mean intensity, each containing mean intensities in one frequency point for all depths,

$$\delta \mathbf{J}_i \equiv \{\delta J_{1i}, \delta J_{2i}, \dots, \delta J_{ND,i}\}, \quad i = 1, \dots, NF, \tag{128}$$

and analogously for the vector of temperatures

$$\delta \mathbf{T} \equiv \{\delta T_1, \delta T_2, \dots, \delta T_{ND}\}. \tag{129}$$

In the description of the method presented in Hubeny & Mihalas (2014; § 17.3), an analogous vector $\delta \mathbf{N}$ for the particle number density was introduced, but this is not done in TLUSTY.

The method is designed for LTE models, although it can in principle be used for NLTE models as well, although in that case the convergence of the scheme is usually quite slow. Nevertheless, in some cases it may provide a stable scheme to obtain an intermediate NLTE model, from which one can then more easily converge a NLTE model using the CL or hybrid CL/ALI scheme.

The point is to express all the material state parameters as functions of temperature and density, and then to express the density as a function of temperature, using the equation of state relating density to gas pressure, and keeping the gas pressure fixed in a given iteration step. This procedure is impractical for hot models where the radiation pressure represents a significant fraction of the total pressure, but is quite reasonable for cool models where the radiation pressure is small or negligible. In that case, $P \approx mg + P_0$ [see equation (11)], and since m is used as the basic depth coordinate, the gas pressure is essentially a known quantity.

The linearized radiative transfer equation (for inner depth points) can be written as

$$\sum_{d'=d-1}^{d+1} U_{dd',i} \delta \mathbf{J}_{d'i} + \sum_{d'=d-1}^{d+1} R_{dd',i} \delta \mathbf{T}_{d'} = E_{di}, \tag{130}$$

for $i = 1, \ldots, NF$. In the matrix notation

$$\mathbf{U}_i \delta \mathbf{J}_i + \mathbf{R}_i \delta \mathbf{T} = \mathbf{E}_i, \tag{131}$$

where $\mathbf{U}_i$ and $\mathbf{R}_i$ are $ND \times ND$ tridiagonal matrices that account for coupling of the corrections to the radiation field at frequency ν_i and material properties as functions of T, at the three adjacent depth points $(d-1, d, d+1)$. Analogously, the contribution to the linearized energy equation from each frequency i at depth point d is of the form

$$\sum_{i=1}^{NF} \mathbf{V}_i \delta \mathbf{J}_i + \mathbf{W} \delta \mathbf{T} = \mathbf{F}, \tag{132}$$

where $\mathbf{V}_i$ and $\mathbf{W}$ are generally bi-diagonal matrices (in the differential form of the radiative equilibrium; for the integral form they would be diagonal).

The overall structure here is reversed from the original variant, in the sense that the role of frequencies and depths is reversed. The global system is a block-diagonal (since the frequency points are not coupled), with an additional block ("row") with the internal matrices being tridiagonal. Corrections of mean intensities are found from Eq. (131),

$$\delta \mathbf{J}_i = \mathbf{U}_i^{-1} \mathbf{E}_i - (\mathbf{U}_i^{-1} \mathbf{R}_i) \delta \mathbf{T} \tag{133}$$

substituting Eq. (133) into (132), one obtains for the correction of temperature

$$\left(\mathbf{W} - \sum_{i=1}^{NF} \mathbf{V}_i \mathbf{U}_i^{-1} \mathbf{R}_i \right) \delta \mathbf{T} = \left(\mathbf{F} - \sum_{i=1}^{NF} \mathbf{V}_i \mathbf{U}_i^{-1} \mathbf{E}_i \right), \tag{134}$$

which is solved for $\delta \mathbf{T}$., and then $\delta \mathbf{J}_i$ are obtained from Eq. (133).

In this scheme, one has to invert NF tridiagonal; matrices $\mathbf{U}_i$, which is very fast, plus one inversion of the $ND \times ND$ grand matrix in Eq. (134), which is also fast. Since the computer time scales linearly with the number of frequency points, the method can be used even for line-blanketed models.

As stated above, the method is designed for LTE models, but experience shows that the Rybicki scheme can also be applied to NLTE models. The scheme is in this case equivalent to the Lambda iteration (because the corrections of level populations and electron density are not solved simultaneously with the corrections of temperature and radiations field), so it converges very slowly. However, the method is quite stable and it may help avoid divergences that sometimes plague traditional linearization methods. Therefore, although the Rybicki scheme is not a viable option to construct well converged NLTE models, it can be used for getting an intermediate model from which the full NLTE can be converged more easily.

3.4 Acceleration methods

There are three numerical schemes offered by TLUSTY that belong to the category of mathematical *acceleration of convergence*. They are discussed in detail

in Hubeny & Mihalas (2014; § 18.4).

(1) The simplest possibility is the so-called *Kantorovich method* (Hubeny & Lanz 1992). The scheme keeps the Jacobian fixed after a certain iteration, so the subsequent iterations of complete linearization use the same Jacobian (more accurately the inverse of the Jacobian is kept fixed for future use); only the right–hand–side vectors $\mathbf{L}$ are re-evaluated after each iteration. Experience with the method shows that it is surprisingly robust. Usually, one needs to perform a few (3-5) iterations of the full linearization scheme, depending on the problem at hand and the quality of the initial estimate. Also, it is sometimes very advantageous to "refresh" the Jacobian (i.e., set it using the current solution and invert it) after a certain number of Kantorovich iterations. The detailed setup is controlled by input data.

(2) *Ng acceleration* is a very popular acceleration scheme used in conjunction of an ALI scheme for solving a radiative transfer problem (Auer 1984; Olson, Auer, & Buchler 1986). In the context of accelerating a complete–linearization–based scheme to calculate model stellar atmospheres was applied in Hubeny & Lanz (1992).

The general idea is to construct a new iterate of the state vector based on the information not only from the previous iteration step, as in a standard version of an iterative linearization procedure, but also from still earlier steps. While the number of earlier steps may vary, essentially all astrophysical applications use the three–point version. Denoting $\mathbf{x}$ the collection of all state vectors ψ_d at all depth points d, the "accelerated" iterate is written as a linear combination of the three previous iterates,

$$\mathbf{x}^* = (1 - a - b)\mathbf{x}^{(n-1)} + a\mathbf{x}^{(n-2)} + b\mathbf{x}^{(n-3)}, \tag{135}$$

where coefficients a and b are given by

$$a = \left(\delta_{01}\delta_{22} - \delta_{02}\delta_{21}\right) / \left(\delta_{11}\delta_{22} - \delta_{12}\delta_{21}\right), \tag{136}$$
$$b = \left(\delta_{02}\delta_{11} - \delta_{01}\delta_{21}\right) / \left(\delta_{11}\delta_{22} - \delta_{12}\delta_{21}\right), \tag{137}$$

where

$$\delta_{ij} \equiv \left(\Delta\mathbf{x}^{(n)} - \Delta\mathbf{x}^{(n-i)}\right) \cdot \left(\Delta\mathbf{x}^{(n)} - \Delta\mathbf{x}^{(n-j)}\right), \tag{138}$$

for $i = 0, 1, 2$, and $j = 1, 2$; and

$$\Delta\mathbf{x}^{(n)} \equiv \mathbf{x}^{(n)} - \mathbf{x}^{(n-1)}. \tag{139}$$

The scalar product in equation (138) is defined as

$$\mathbf{x} \cdot \mathbf{y} \equiv \sum_{d=1}^{ND} \sum_{i=1}^{NN} W_{di} x_{di} y_{di}, \tag{140}$$

where W_{di} is a weighting factor, taken in TLUSTY as $W_{di} = 1/\psi_{di}$. Experience has showed that in a large majority of cases the Ng acceleration improves convergence significantly; the acceleration is usually performed for the first time at

or around the 7-th iteration of the linearization scheme, and is done typically every 4 iterations afterwards. Again, the detailed setup is driven by input data – see Paper III, § 7.4.8. In some cases, like in models with convection, or in specific models with sharp ionization fronts, the Ng acceleration does not help, and may even lead to numerical problems and divergence. Therefore, one should apply the Ng acceleration judiciously.

(3) Successive over–relaxation (SOR). It consists in multiplying the corrections $\delta\psi$ by a certain coefficient α. This coefficient can be either set by an educated guess, or one can use the procedure suggested by Trujillo-Bueno & Fabiani-Bendicho (1995), namely to express α in terms of the spectral radius of the appropriate iteration operator, which in turn may be approximated by a ratio of maximum relative changes of the source function in the two subsequent previous iterations.

3.5   Treatment of opacities

The opacities are treated in TLUSTY in several different ways:

(1) The current opacities and emissivities are evaluated on the fly for the current structural parameters (temperature, density, atomic level populations). This is a traditional approach, which is moreover mandatory for NLTE models. In this approach, the absorption and emission coefficients are evaluated essentially by using their definition equations (87) and (90). The actual transitions that contribute to the total opacity are specified through selecting atomic species, ions, and levels which are called "explicit". Therefore, the transitions between explicit levels of explicit ions of explicit atoms do contribute to the total opacity. The opacity (emissivity) of an individual explicit transition is a function of level populations of the lower and upper states, and the corresponding cross section which in turn is a function of structural parameters such as temperature, electron density, and possibly others. Since all these quantities are being updated during the iteration process, the opacity/emissivity is recalculated again and again.

(2) A variant of this approach is the opacity and emissivity of "superlines", that is, transitions between "superlevels". A superlevel is a set of individual energy levels that are assumed to have the same NLTE departure coefficient or, in other words, are in LTE within each other. For details, refer to § 3.6. As explained there, relevant cross sections are evaluated at the beginning and are held fixed afterward. Nevertheless, the corresponding superlevel populations are being updated, so the corresponding opacities are still being re-evaluated during the iteration process.

(3) As indicated in equations (86) and (90), TLUSTY also allows for the so-called additional opacities. These are typically transitions between upper levels of explicit species that are not treated explicitly, and also H_2^+ or H^- opacity (if the H^- ion is not treated explicitly) The user has an option to include more additional opacities by means of adding corresponding expressions to a previously provided subroutine. In all these cases, the corresponding cross

sections are taken as analytic expressions, or from simple tables.

(4) While the above procedure is unavoidable for NLTE models, it is not efficient for LTE models, where the opacity depends only on temperature and density, and emissivity is given through the Kirchhoff-Planck relation, $\eta_\nu = \kappa_\nu B_\nu$, In the past, LTE models were considered, within the context of TLUSTY applications, just as intermediate models which provide suitable starting models for the NLTE ones. However, once the range of applications of TLUSTY extended to cool and very cool objects, such as the lower end of the main sequence, brown dwarfs, and planetary atmospheres, LTE models, with possible additional complexities such as molecular and cloud opacities, become important on their own merit.

In this case, it is much more efficient to pre-calculate extensive tables of opacity as a function of frequency, temperature, and density (or electron density). In an actual run of TLUSTY, one simply interpolates from the tabular values of opacity to the current values of structural parameters and frequency. Such an approach has been used in a previously separate variant of TLUSTY called CoolTLUSTY (e.g. Hubeny, Burrows, & Sudarsky 2003), and was extensively used for computing model atmospheres of brown dwarfs and extrasolar planets.

Starting with version 204, such an approach has been adopted in the mainstream TLUSTY as well. We do not use tables constructed specifically for substellar mass objects (Sharp and Burrows 2007) because they are not released for public distribution. However, we have constructed opacity tables for temperatures between 3,000 and 10,000 K, so that one can use these tables to compute LTE model atmospheres for F and G type stars. The current tables do not contain molecular opacities. Currently, we are working on preparing more extensive opacity tables, including molecular and cloud opacities, applicable for the whole range of parameters.

In this approach one does not need to select explicit atoms, ions, levels, and transitions, because the opacities are given and the kinetic equilibrium equations are not solved. There is a choice how to treat the equation of state and to evaluate the necessary thermodynamic parameters needed to describe convection. This can be done either on the fly, in which case one has to supply data for implicit species (abundances, a mode of evaluation of the partition functions), or by interpolating in additional pre-calculated tables that specify the equation of state (essentially a relation between density and pressure), and also other thermodynamic variables needed to evaluate the convective flux – see Paper III, § 13.1.

(5) Finally, there is a hybrid approach, in which some opacities (or bulk of opacities) are treated explicitly (options 1 – 3 above), while the remaining opacity sources, presumably less important ones, or those for which LTE is a good approximation (such as molecular opacities) are treated by means of an opacity table. Such an approach is already coded in TLUSTY, Version 205, but an evaluation of the corresponding partial opacity tables was not yet fully streamlined.

3.6 Superlevels and superlines

Using the hybrid CL/ALI method, the number of frequency points can be reduced dramatically. However, the number of explicit levels needed for NLTE metal line-blanketed model atmospheres may still be enormous. For instance, each ion of Fe has of the order 10^4 energy levels.

To deal with this problem, one introduces the concept of a superlevel. The idea consists of grouping several, possibly many, individual energy levels together, forming a *superlevel*. The basic physical assumption is that all genuine levels j within a superlevel J are in Boltzmann equilibrium with respect to each other,

$$n_j/n_{j'} = g_j/g_{j'} \exp[-(E_j - E_{j'})/kT]. \tag{141}$$

Therefore, the whole superlevel can be treated as one level for solving the kinetic equilibrium equation. There is a certain flexibility in choosing a partitioning of levels into superlevels. However, in order to provide a realistic description, the levels forming a superlevel have to possess close energies, and to have similar properties, for instance belonging to the same multiplet, the same spin system, or having the same parity. The requirement of close energies is needed because collisional rates between levels with a small energy difference tend to be large and hence dominate over the radiative rates. With dominant collisional rates, one indeed recovers LTE.

As mentioned in § 2.1, we have introduced also a special kind of superlevels, called *merged levels*. They behave like normal superlevels, the only differences are (i) they are introduced only for the higher states of hydrogen and hydrogenic ions, and (ii) therefore, their parameters, and the necessary cross sections for transition involving them are computed analytically, without a need of additional data.

Bound-bound transition involving at least one superlevel are called superlines. The absorption coefficient for a transition $I \rightarrow J$, not corrected for stimulated emission, is given by

$$\kappa_{IJ}(\nu) = \sum_i \sum_j n_i w_j \sigma_{ij}(\nu), \tag{142}$$

where $\sigma_{ij}(\nu) = (\pi e^2/m_e c) f_{ij} \phi_{ij}(\nu)$, is the cross section for the transition $i \rightarrow j$, f_{ij} is the oscillator strength, and $\phi_{ij}(\nu)$ the (normalized) absorption profile coefficient, n_i and w_j are the population of the lower level, and the occupation probability of the upper level, respectively.

Within the superlevel formalism, the absorption coefficient for transition $I \rightarrow J$ has to be given by [for details, refer to Hubeny & Mihalas (2014, § 18.5)]

$$\kappa_{IJ}(\nu) = n_I w_J \sigma_{IJ}(\nu); \tag{143}$$

therefore the cross section is given by

$$\sigma_{IJ}(\nu) = \frac{g_I \exp(-E_J/kT) \sum_i \sum_j g_i w_i w_j \sigma_{ij}(\nu) \exp(-E_i/kT)}{\left[\sum_i g_i w_i \exp(-E_i/kT) \right] \left[\sum_j g_j w_j \exp(-E_j/kT) \right]}, \tag{144}$$

and

$$w_J = \frac{\exp(E_J/kT)}{g_J} \sum_j g_j w_j \exp(-E_j/kT). \qquad (145)$$

which has the meaning of generalized occupation probability for superlevel J. It should be noted that in general $w_J \neq 1$ even if one sets all the occupation probabilities of the components j to $w_j = 1$.

Since the number of individuals levels forming a superlevel may be quite large (of the order of several tens to several hundreds), and so the number of individual lines forming a superline may be huge (say, of the order of 10^4 to 10^5, or perhaps even more), the resulting superline cross section is a rather complicated function of frequency. It would be impractical to compute it for every depth point independently; moreover the amount of necessary atomic data (the individual oscillator strengths, the line broadening parameters) will also be impractically large. Therefore, the superline cross sections are evaluated at the beginning of a given TLUSTY run, and subsequently held fixed, for several depth points (typically 3, but this number is a free parameter and can be changed if needed). For other depth points, they are interpolated. As stated in §.2.5, the cross sections to be used in TLUSTY are evaluated by means of the so-called Opacity Sampling (OS), that is at frequency points that are set by the code to cover the whole range of a superline, and with a frequency spacing that is given by a certain multiple of a fiducial Doppler width[1]. This spacing is also a free parameter. For most accurate models (such as the OSTAR2003 and BSTAR2007 grids of NLTE line-blanketed model atmospheres of O and B stars – Lanz & Hubeny 2003; 2007), the spacing was taken as 0.75, but it can be taken much higher; as shown in Lanz & Hubeny (2003), even vales such as 40-50 produce reasonably accurate model atmospheres.

In the past, the superline cross sections were treated by means of the Opacity Distribution Function (ODF) – see Hubeny & Lanz (1995), which uses a resampled cross section that is represented by a low number of frequency points. However, this option is not accurate enough because it does not treat the overlaps of superlines properly. Also, it requires additional input files that contain the tabulated ODF values. Although it is still offered in TLUSTY, it is not recommended.

The superline cross sections are computed at the beginning of the calculation based on data from Kurucz files, for instance, for Fe II the files `gf2601.gam` and `gf2601.lin`. The former file contains parameters for the individual energy levels (energy, statistical weight, quantum numbers), while the latter contains the data for individual lines (oscillator strengths, broadening parameters).

The concept of an ODF is also used for treating the opacity in a transition form a regular level to a merged level in the case of hydrogen and hydrogenic ions. In this case, however, the ODF is constructed on the fly because the cross sections for the individual lines forming such a superline can be computed analytically. Some additional input parameters to construct such an ODF are

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[1] Fiducial Doppler width is defined as a Doppler width for Fe corresponding to the effective temperature

described in Paper III, § 11.3. However, even this option is somewhat obsolete, as it is possible to treat the hydrogen atom with many explicit levels (say, 16 or more), in which case the higher levels are mostly dissolved, and the opacity in the transitions from lower levels into the merged level are described through the pseudocontinuum opacity.

3.7 Level grouping and zeroing

Another procedure, which may significantly reduce the number of level populations to be linearized is the idea of *level grouping*. A level group is a set of several levels whose populations are assumed to vary in a coordinated way in the linearization. More precisely, instead of linearizing individual level populations, one linearizes the total population of the group, assuming that the ratios of the individual level populations within the group to the total population of the group are unchanged during a current linearization step. In the formal solution step, one solves the kinetic equilibrium equations for all the individual level populations.

The concept of level groups should not be confused with the concept of superlevels; in the former case, the level groups are only a numerical trick to make the complete linearization matrices smaller, while the level populations are determined exactly; the latter case—superlevels—approximates the individual populations of the components of the superlevel by assuming that they are in Boltzmann equilibrium with respect to each other. In fact, one may group the individual superlevels into level groups as well.

Another numerical trick used in TLUSTY is a *level zeroing*. For each depth point, the code examines a ratio of level populations to the total population of an ion. If this value decreases below a certain value (a free parameter, typically taken 10^{-20}), the level population of such a level is set to zero, and the kinetic equilibrium equation for such particular depth point is written as $n_i = 0$ (that is, in a matrix form, $A_{ii} = 1$, $A_{ij} = 0$ for $i \neq j$, and $b_i = 0$). The level still remains in the set of explicit level since its population might be non-negligible or even significant in other depth points. If, however, the population would be zeroed in all depth points, the level is completely removed from the set of explicit levels. This procedure helps to improve a numerical stability of the system, avoids solving for level populations which are of no practical interest, and also allows the user to use relatively general atomic data sets with many ions.

3.8 Formal solution

The term "formal solution" is used in two different meanings:

(i) In a limited context, the "formal solution of the transfer equation" means a solution of this equation for one frequency at a time, with the *specified source function*. At this step the Eddington factors are being evaluated.

(ii) The set of all calculations between two iterations of the global iteration (i.e., linearization) scheme. In the standard case, it means a simultaneous so-

lution of the radiative transfer and kinetic equilibrium equations, keeping the values of other state parameters (temperature, density, electron density) fixed at the current values. Depending on the setup of the run, it may also include the recalculation of other state parameters, such as electron density, or mass density, or even temperature. The point of this procedure is to help the global iteration scheme to converge faster by improving the values of the state vector as much as possible before entering the next iteration step. It will be called here *global formal solution.*

3.8.1 Formal solution of the transfer equation

TLUSTY offers several types of the formal solution which are selected by means of input data. A detailed description of the schemes is presented in Hubeny & Mihalas (2014; § 12.4).

Briefly, discretizing in frequency and angle, the transfer equation is written as

$$\mu_m \frac{dI_{nm}}{d\tau_n} = I_{nm} - S_n \qquad (146)$$

where I_{nm} is the specific intensity at frequency point n and angle point m; μ_m is the cosine of the polar angle. S_n is the source function, given by

$$S_n = \frac{\kappa_n}{\chi_n} + \frac{\sigma_n}{\chi_n} \sum_{m'} w_{m'} I_{nm'}. \qquad (147)$$

The last term represents the scattering part of the source function, assuming isotropic and coherent scattering (e.g. Thomson electron scattering; the case of non-coherent Compton scattering is described in Paper III, § 12.5); w_m are the angular quadrature weights.

The default method of solution is the Feautrier method that introduces symmetric and antisymmetric averages of the specific intensity, more specifically $j_{nm} \equiv [I_n(\mu_m) + I_n(-\mu_m)]/2$, and $h_{nm} \equiv [I_n(\mu_m) - I_n(-\mu_m)]/2$, and rewrites the transfer equation (146) in a second-order form,

$$\mu_m^2 \frac{d^2 j_{nm}}{d\tau_n^2} = j_{nm} - \frac{\kappa_n}{\chi_n} - \frac{\sigma_n}{\chi_n} \sum_{m'=1}^{NA} w_{m'} I_{nm'}, \qquad (148)$$

where NA is the number of angle points in one hemisphere ($\mu > 0$). This equation is supplemented by the boundary conditions

$$\mu_m \left. \frac{dj_{nm}}{d\tau_n} \right|_0 = j_{nm}(0) - I_{nm}^{\text{ext}}, \qquad (149)$$

where I_{nm}^{ext} is the incoming specific intensity $I(\nu_n, -\mu_m)$. Equation (149) is only first-order accurate. Auer (1967) suggested a convenient second-order from which is based on a Taylor expansion

$$j_{nm}(\tau_{2,n}) = j_{nm}(\tau_{1,n}) + \Delta\tau_{3/2,n} \left. \frac{dj_{nm}}{d\tau_n} \right|_1 + \frac{1}{2}(\Delta\tau_{3/2,n})^2 \left. \frac{d^2 j_{nm}}{d\tau_n^2} \right|_1, \qquad (150)$$

which is used to achieve a second-order accuracy,

$$\mu_m \frac{j_{nm}(\tau_{2n}) - j_{nm}(\tau_{1n})}{\Delta \tau_{3/2,n}} = j_{nm}(\tau_{1n}) + \Delta \tau_{3/2,n} \frac{j_{nm}(\tau_{1n}) - S_n(\tau_{1n})}{2\mu_m}. \qquad (151)$$

and for the lower boundary

$$\mu_m \left. \frac{dj_{nm}}{d\tau_n} \right|_{\tau_{\max}} = I_{nm}^+(\tau_{\max}), \qquad (152)$$

where $I_{nm}^+(\tau_{\max})$ is the outward-defected specific intensity at the deepest point, given either by the diffusion approximation (for stellar atmospheres)

$$I_{nm}^+(\tau_{\max}) = B(\nu_n, \tau_{\max}) + \mu_m \left. \frac{\partial B(\nu_n)}{\partial \tau_{\nu_n}} \right|_{\tau_{\max}}, \qquad (153)$$

or by a symmetric lower boundary condition (for accretion disks)

$$\mu_m \left. \frac{dj_{nm}}{d\tau_n} \right|_{\tau_{\max}} = 0. \qquad (154)$$

All frequency points in Eqs. (148) – (154) are independent, so that they can by solved for one frequency at a time. We skip the frequency index n and discretize in depth, described by index d. One introduces a column vector $\mathbf{j}_d \equiv (j_{d,1}, j_{d,2}, \ldots, j_{d,NA})$, and writes Eqs. (148) – (154) as a linear matrix equation

$$-\mathbf{A}_d \mathbf{j}_{d-1} + \mathbf{B}_d \mathbf{j}_d - \mathbf{C}_d \mathbf{j}_{d+1} = \mathbf{L}_d, \qquad (155)$$

where $\mathbf{A}_d$, $\mathbf{B}_d$, and $\mathbf{C}_d$, are $NA \times NA$ matrices; $\mathbf{A}$ and $\mathbf{C}$ are diagonal, while $\mathbf{B}$ is full. The system is solved by the standard Gauss-Jordan elimination, equivalent to Eqs. (123) - (125). In terms of j, the mean intensity and the Eddington factor are given by

$$J_n = \sum_{m=1}^{NA} w_m j_{nm}, \quad \text{and} \quad f_n = \sum_{m=1}^{NA} w_m \mu_m^2 j_{nm} \Big/ J_n. \qquad (156)$$

The program offers several variants of the Feautrier scheme: scheme

- ordinary second–order Feautrier (1964) scheme;
- improved scheme by Rybicki & Hummer (1991);
- spline collocation scheme (Mihalas & Hummer (1974);
- Auer (1976) fourth-order Hermitian scheme.

By the nature of the Feautrier scheme, all these methods solve the transfer equation for one frequency, but all angle points, at a time. This involves solving the transfer equation for vectors of specific intensities for all angles (with number NA, with a need of inverting a number of $NA \times NA$ matrices. Since the typical value of NA is quite low ($NA = 3$ by default, which corresponds to 6 actual discretized angles) inverting such matrices does not present any problem or any

appreciable time consumption. The basic advantage of the Feautrier scheme is that it treats scattering directly, without any need to iterate.

However, if the number of angles is large (for as comparison purposes, or some very specific applications), or if an atmospheric structure exhibits very sharp variations with depth (e.g., sharp ionization fronts), it is advantageous to use another offered scheme:

• Discontinuous Finite Element (DFE) scheme by Castor, Dykema, & Klein (1992). It solves the linear transfer equation (146) directly for the specific intensity, and therefore if scattering is present, which is essentially always, the scattering part of the source function has to be treated iteratively. To this end, a simple ALI-based procedure is used; its setup is described through the corresponding input parameters – see Paper III, § 7.4.3 and § 13.1.

3.8.2 Global formal solution

The main part of the global formal solution is a simultaneous solution of the radiative transfer equation and the set of kinetic equilibrium equations for all explicit levels. Notice that in this step the levels that form a group that is linearized as a single level are now treated separately, so that the populations of the individual levels in the group are updated.

This is a typical NLTE line formation problem. The main point is that the solution does not have to be perfect; it is only supposed to provide a somewhat more consistent values of level populations and radiation intensities before entering the next global iteration step. Therefore, in the past, one employed several ordinary Lambda iterations, that is, an iterative solution that alternates between solving the transfer equation for the current values of level populations, and solving the kinetic equilibrium equations with the current values of radiation intensities.

Later, this procedure was upgraded to treat the coupled problem more efficiently using the ALI technique together with preconditioning, developed by Rybicki & Hummer (1991, 1992); for a description see Appendix B1, and for more details refer to Hubeny & Mihalas (2014; § 14.5). This scheme offers an interesting possibility to solve the so-called restricted NLTE problem (line formation with fixed atmospheric structure), without a linearization, provided that one allows for enough iterations of the global formal solution step. We recall that there are several computer programs designed specifically for this problem – the "Kitt Peak code" of Auer (1973), PANDORA (Avrett & Loeser 1982), MULTI (Carlsson 1986), DETAIL/SURFACE (Butler & Giddings 1978) and others.

In parallel with, or on top of, this procedure, one can perform other "formal" solutions, essentially updating one state parameter by solving the appropriate equation, while keeping other state parameters fixed. These include:
– updating electron density by solving the charge conservation equation;
– updating pressure by solving the hydrostatic equilibrium equation;
– updating temperature, by solving the radiative (or radiative + convective) equilibrium equation.

A particularly important set of procedures is devised for models with convection, where in the global formal solution step one has to iteratively improve the temperature and other state parameters to smooth the solution that follows directly from the previous iteration step. In many cases, not using such procedures would have disastrous consequences for the convergence properties, or even lead to a violent divergence of the iteration scheme. These procedures will be described in Appendix B2.

3.9 Discretization parameters

As stated above, the program is fully data-oriented. Both the genuinely discrete quantities, (number of explicit atoms, ions, levels, transitions, etc,), as well as discretized quantities (number of depth points, frequency points, etc.), are either set up directly (e.g. the number of depth points), but typically they are being computed by the code based on the actual input. Therefore, they are not known a priori.

Since TLUSTY can be used for a wide range of applications, these numbers can be vastly different for various cases. As described in the next chapter, the code can be compiled differently for different applications in such a way that it does not require an unreasonable amount of core memory, and still reflects the needs based on the selected setup.

We list most of these important numbers below, using the names trey are referred to in the TLUSTY source code.

NATOM – number of explicit atoms. Each explicit atom is composed of one or several ionization stages, called explicit ions. The highest ionization stage has to be considered as a one-level ion.

NION – number of explicit ions. The highest ionization stage is *not* counted in the number of explicit ions.

NLEVEL – number of explicit levels, defined such as these are the energy levels for which the kinetic equilibrium equation is being solved, and whose populations can therefore depart from their LTE values. The one-level highest ions of the explicit species are now counted into the total number of levels. The individual superlevels and merged levels are counted as one level each.

NLVEXP – number of explicit levels whose populations are linearized. This number is equal to NLEVEL if all levels are treated individually, but is lower than NLEVEL if one introduces level groups. In many cases, NLVEXP is significantly lower that NLEVEL; for instance in the example in Paper III, § 6.3, NLEVEL=1127 while NLVEXP=222 (there, we show them as MLEVEL and MLVEXP in an output from the code PRETLUS where they represent the actual values of these parameters for the given model).

NTRANS – number of transitions, both bound-bound and bound-free, between explicit energy levels. All transitions that are somehow taken into account are counted into this number even if they are set in detailed radiative balance or are dipole-forbidden, since in both these cases, the collisional rates still have non-zero values.

ND – number of discretized depth points

NFREQ – the total number of discretized frequency points. Since the selection of frequencies is very important for the overall accuracy of the resulting model, the selection of frequency points is set by the program based a number of input parameters – see Paper III, §7.4.2. When computing metal line–blanketed models with a large number of superlevels and superlines, the program first sets the frequency points independently for each line and superline, and computes the corresponding cross section in these frequencies. Since there is typically a large number of line overlaps, the program then removes some unnecessary points originating from line overlaps.

NFREQP – the number of auxiliary frequency points in the original setup. This number is typically larger than MFREQ, and the reason that is kept separate is that there are only a few arrays in the code that have to have dimension NFREQP or larger, while there is a number of arrays, many of them multidimensional, for the final set of frequencies with number NFREQ,

NFREQC – number of frequency points in the continua. This set contains the frequencies that do not specifically belong to any line, although the opacity of some wide lines (e.g. Lyman α) may still contribute to the total opacity in such frequencies.

NFREX – number of frequency points in which the mean intensity is linearized. When using the hybrid CL/ALI method, this number is significantly smaller than NFREQ.

NFREQL – the maximum number of frequency points per line.

NTOT≡NN – the dimension of the state vector ψ, that is, the number of the state parameters. It is given by NFREX+NLVEXP+NC, where NC is the number of structural parameters other than the mean intensities and level populations that are linearized. As explained in §3.1, NC can attain values between 0 (when the atmospheric structure is held fixed), to 6 (for accretion disk with convection and with including fictitious massive particle density; the physical quantities then being T, N, n_e, n_m, z, and ∇). A typical value for stellar atmospheres is 3, for T, N, and n_e.

NMU – number of angle points for the formal solution of the transfer equation and determination of the Eddington factor. Its default value is 3, but can be changed by an appropriate input parameter – see Paper III, §7.4.6.

There are several secondary numbers that specify the sizes of some multi-dimensional arrays. (The lengths of 1-dimensional arrays are not important; they may oversized to satisfy the requirements following from any physical setup without causing memory problems). They include the following:

NLINES(IJ) - number of lines that contribute to the opacity at frequency point IJ (that is, the total number of line overlaps at frequency IJ)

NBF – the number of bound-free transitions

NFIT – the maximum number of fit points for the input of the photoionization cross sections when using the Opacity Project data.

NCDW – number of levels with pseudocontinua

NMER – number of merged levels

NVOIGT – number of lines with a Voigt profile

There are also several arrays that are set only for the treatment of superline cross sections, that is, when computing metal line-blanketed models. These arrays may be rather big and take a lot of memory. It it not advised to set them to the maximum values for all kinds of models. The dimensions of these files are the following:

NDODDF – number of depth points for storing the superline cross sections.

NKULEV – the maximum number of internal energy levels for an ion treated with superlevels. The data for these levels are read from Kurucz files, e.g. `gf2601.gam` for Fe II.

NLINE – number of internal (genuine) lines for an ion; data for them are read from Kurucz files, e.g. `gf2601.lin` for Fe II. Based on these data, the superline cross sections are constructed.

NCFE – the total number of internal frequency points used for computing and storing the cross section or the individual lines, from which the superline cross section is constructed.

4 Initial LTE-gray model

4.1 Stellar atmospheres

The procedure to construct the initial LTE-gray model is very similar to that described by Kurucz (1970).

One first sets up a scale in the Rosseland optical depth, typically logarithmically equidistant between τ_1 and τ_D, which are input parameters of the model construction; typically chosen $\tau_1 \approx 10^{-7}$ and $\tau_D \approx 10^2$. Temperature is a known

function of the Rosseland optical depth (e.g. Hubeny & Mihalas 2014, $17.2 and 17.7):

$$T^4(\tau) = (3/4)T_{\mathrm{eff}}^4[\tau + q(\tau)] + (\pi/\sigma_R)H^{\mathrm{ext}} \tag{157}$$

where $q(\tau)$ is the Hopf function, and $H^{\mathrm{ext}} = \int_0^\infty H_\nu^{\mathrm{ext}} d\nu$ is the frequency-integrated external irradiation flux.

The hydrostatic equilibrium equation is written as

$$\frac{d\ln P}{d\ln \tau} = \frac{g\tau}{\kappa P}, \tag{158}$$

because τ and P span many orders of magnitude, so it is advantageous to integrate the equation for logarithms. Here κ is the Rosseland mean opacity.

The total pressure $P = P_{\mathrm{gas}} + P_{\mathrm{rad}}$ (we neglect the turbulent pressure here). The radiation pressure is expressed as follows: Its gradient can be approximated as

$$dP_{\mathrm{rad}}/d\tau \approx (4\pi/c)\int_0^\infty (dK_\nu/d\tau_\nu)\,d\nu = (4\pi/c)\int_0^\infty H_\nu d\nu = (\sigma_R/c)T_{\mathrm{eff}}^4, \tag{159}$$

where the first equality follows from Eq. (14), and the last one from the definition of the effective temperature. The radiation pressure is thus given by

$$P_{\mathrm{rad}}(\tau) = (\sigma_R/c)T_{\mathrm{eff}}^4\tau + P_{\mathrm{rad}}^0, \tag{160}$$

where P_{rad}^0 is the radiation pressure at the surface. Using the Eddington approximation $[K_\nu = (1/3)J_\nu$, and $H_\nu^0 = (1/\sqrt{3})J_\nu^0]$, it is approximated by

$$P_{\mathrm{rad}}^0 = (4\pi/c)\int_0^\infty K_\nu d\nu \approx (\sigma_R/c)(1/\sqrt{3})\,T_{\mathrm{eff}}^4. \tag{161}$$

One then proceeds by solving Eq. (159) from the top of the atmosphere to the bottom. At the first depth point, τ_1, one makes a first estimate of the Rosseland mean opacity, κ_1, and assuming it is constant from this point upward, and using the boundary condition $P_{\mathrm{gas}}(0) = 0$, one obtains the first estimate of the total pressure,

$$P_1 = (g/\kappa_1)\tau_1 + P_{\mathrm{rad}}^0. \tag{162}$$

Having an estimate for the total pressure, one uses the following procedure which is valid for every depth point d:

- from current total pressure P_d, at depth point d, one first extracts the gas pressure, $P_{\mathrm{gas}} = P - (\sigma_R/c)T_{\mathrm{eff}}^4\tau_d - P_{\mathrm{rad}}^0$;

- from the known temperature $T(\tau_d)$, given by Eq. (157), we compute the total particle number density $N = P_{\mathrm{gas}}/(kT)$;

- with known T and N, one determines the electron density n_{e} by solving the set of Saha equations and the charge equilibrium equation;

- with known T and n_e, one computes LTE level populations of all explicit levels of all explicit ions;

- using these level populations, one computes monochromatic opacities for all selected frequency points, and consequently the new value of the Rosseland mean opacity κ from its definition,

$$\frac{1}{\kappa} = \frac{\int_0^\infty (1/\chi_\nu)(dB_\nu/dT)\, d\nu}{(dB/dT)}. \tag{163}$$

We will refer to this procedure as $P \to \kappa$. With the new value of κ, one returns to Eq. (162), evaluates an improved estimate of P_1, and repeats the procedure $P \to \kappa$ until convergence. Once this is done, one proceeds to the next depth point.

For the next three depth points, $d = 2, \ldots, 4$, one obtains the first estimate (a predictor step) of the total pressure by:

$$\ln P_d^\mathrm{pred} = \ln P_{d-1} + \Delta \ln P_{d-1}, \tag{164}$$

which is followed by a $P \to \kappa$ procedure, and with the new κ one goes to the corrector step,

$$\ln P_d = (\ln P_d^\mathrm{pred} + 2 \ln P_{d-1} + \Delta \ln P_d + \Delta \ln P_{d-1})/3, \tag{165}$$

where

$$\Delta \ln P_d = \frac{g \tau_d}{\kappa_d P_d}(\ln \tau_d - \ln \tau_{d-1}). \tag{166}$$

For the subsequent depth points, one uses the Hamming's predictor-corrector scheme (see Kurucz 1970), where the predictor step is

$$\ln P_d = (3 \ln P_{d-4} + 8 \ln P_{d-1} - 4\Delta \ln P_{d-2} + 8\Delta \ln P_{d-3})/3, \tag{167}$$

and the corrector step

$$\ln P_d = (126 \ln P_{d-1} - 14 \ln P_{d-3} + 9 \ln P_{d-4} + 42\Delta \ln P_d$$
$$+ 108\Delta \ln P_{d-1} - 54\Delta \ln P_{d-2} + 24\Delta \ln P_{d-3})/121. \tag{168}$$

After completing the above procedure for all depths, one constructs the column mass scale, which will subsequently be used as the basic depth scale, as

$$m_d = (P_d - P_\mathrm{rad}^0)/g. \tag{169}$$

When convection is taken into account, one first computes the radiative gradient of temperature,

$$\nabla_{\mathrm{rad},d} = \frac{(T_d - T_{d-1})}{(P_d - P_{d-1})} \frac{(P_d + P_{d-1})}{(T_d + T_{d-1})}, \tag{170}$$

and compares to the adiabatic gradient, ∇_add. If $\nabla_\mathrm{rad} > \nabla_\mathrm{add}$, the criterion for stability against convection is violated, we must determine the true gradient ∇,

where $\nabla_{\mathrm{ad}} \leq \nabla \leq \nabla_{\mathrm{rad}}$, that gives the correct total, radiative plus convective, flux. If the instability occurs deep enough for the diffusion approximation to be valid, then $(F_{\mathrm{rad}}/F) = (\nabla/\nabla_{\mathrm{ad}})$, and the energy balance equation reads (see Hubeny & Mihalas 2014, §17.4),

$$\mathcal{A}(\nabla - \nabla_{\mathrm{el}})^{3/2} = \nabla_{\mathrm{rad}} - \nabla, \tag{171}$$

where ∇_{el} is the gradient of convective elements, and

$$\mathcal{A} = (\nabla_{\mathrm{rad}}/\sigma_{\mathrm{R}} T_{\mathrm{eff}}^4)(gQH_P/32)^{1/2}(\rho c_P T)(\ell/H_P)^2. \tag{172}$$

We see that $\mathcal{A}$ depends only on local variables. Adding $(\nabla - \nabla_{\mathrm{el}}) + (\nabla_{\mathrm{el}} - \nabla_{\mathrm{ad}})$ to both sides of (171), and using the expression $\nabla_{\mathrm{el}} - \nabla_{\mathrm{ad}} = B\sqrt{\nabla - \nabla_{\mathrm{el}}}$, where B is given by Eq. (22), to eliminate $(\nabla_{\mathrm{el}} - \nabla_{\mathrm{ad}})$, we obtain a cubic equation for $x \equiv (\nabla - \nabla_{\mathrm{el}})^{1/2}$, namely

$$\mathcal{A}(\nabla - \nabla_{\mathrm{el}})^{3/2} + (\nabla - \nabla_{\mathrm{el}}) + B(\nabla - \nabla_{\mathrm{el}})^{1/2} = (\nabla_{\mathrm{rad}} - \nabla_{\mathrm{ad}}). \tag{173}$$

or

$$\mathcal{A}x^3 + x^2 + Bx = (\nabla_{\mathrm{rad}} - \nabla_{\mathrm{ad}}), \tag{174}$$

which can be solved numerically for the root x_0. We thus obtain the true gradient $\nabla = \nabla_{\mathrm{ad}} + \mathcal{B}x_0 + x_0^2$, and can proceed with the integration, now regarding T as a function of P and ∇.

4.2 Accretion disks

The adopted procedure closely follows that described in detail by Hubeny (1990). An evaluation of the LTE-gray model proceeds in three, possibly four, basic steps:

1. Initialization of m, ρ, P, and z.

Unlike the case of stellar atmospheres, one first sets up a column mass scale, based on an empirically chosen m_1, the column mass at the first depth point, and m_0, the column mass at the central plane. The latter is determined as described in §2.2. The individual mass-depth points are set logarithmically equidistant between m_1 and m_0. One then calculates an initial estimate of the density ρ and the vertical distance z corresponding to the column masses m_d, using the following procedure:

One introduces the characteristic gas pressure and radiation pressure scale heights H_g and H_r as

$$H_g = (2c_g^2/Q)^{1/2} \tag{175}$$

$$H_r = (\sigma_R/c)T_{\mathrm{eff}}^4 \kappa/Q, \tag{176}$$

where Q is the gravity acceleration parameter defined by Eq. (54), κ is the Rosseland mean opacity, and c_g is the isothermal sound speed associated to the

gas pressure, $c_g = (P_g/\rho)^{1/2}$. It is generally given by

$$c_g^2 = \frac{k}{\mu m_H} \frac{N}{N - n_e} T, \tag{177}$$

where μ is the mean molecular weight, and m_H is the hydrogen atom mass. The factor $N/(N - n_e)$ accounts for a varying degree of ionization of the material; for a pure-hydrogen gas it attains values between 1 (for completely neutral gas) to $1/2$ (for completely ionized gas).

The sound speed is initially taken as depth-independent, corresponding to the effective temperature, The initial estimate of κ for the first depth point is $\kappa_1 = \sigma_e/(\mu m_H)$. One introduces two dimensionless parameters,

$$r \equiv H_r/H_g, \quad y \equiv H/H_g, \tag{178}$$

where H is a combined scale height, given by the solution of the following transcendental equation

$$y = \frac{\sqrt{\pi}}{2} \left(\frac{y}{y - r} \right)^{1/2} \left\{ 1 - \mathrm{erfc}\left[\sqrt{y(y - r)} \right] \right\} + \mathrm{erfc}(y - r) \exp[-r(y - r)], \tag{179}$$

which is solved by the Newton-Raphson method, with the initial estimate $y_0 = r + (1/r)$ for $r > 1$, and $y_0 = \sqrt{\pi}/2$ for $r \leq 0$. The geometrical distance from the central plane expressed in units of gas pressure scale height, $x \equiv z/H_g$, is given by (Hubeny 1990),

$$x = r + \mathrm{inverfc}\left\{ \frac{m}{m_0} \frac{2y}{\sqrt{\pi}} \exp[r(y - r)] \right\} \quad \text{for } x \leq y, \tag{180}$$

$$x = \sqrt{\frac{y}{y - r}} \mathrm{inverfc}\left\{ \sqrt{\frac{4y(y - r)}{\pi}} \frac{m - m_y}{m_0} + \mathrm{erfc}\left[\sqrt{y(y - r)} \right] \right\} \quad \text{for } x > y, \tag{181}$$

where

$$m_y = m_0 \frac{\sqrt{\pi}}{2y} \exp[r(y - r)] \mathrm{erfc}(y - r), \tag{182}$$

and $\mathrm{inverfc}(x)$ is the inverse complementary error function, which can be evaluated by a suitable fitting formula (see Hubeny 1990).

The first estimate of density is given by

$$\rho(x) = \rho_0 \exp\left[-x^2(1 - r/h) \right] \quad \text{fort } x \leq y, \tag{183}$$

$$\rho(x) = \rho_0 \exp[-(x - r)^2] \exp[-r(y - r)] \quad \text{for } x > y, \tag{184}$$

where ρ_0 is the density at the central plane, $\rho_0 = m_0/(yH_g)$. The initial estimate of the gas pressure is then obtained using the sound speed for the characteristic temperature, $P_g(m) = c_g^2 \rho(m)$. Finally, the initial estimate of the vertical distance from the central plane is obtained by solving the z-m relation, $dz = -dm/\rho$.

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2. Initial estimate of the temperature.

The procedure differs depending on whether or not the Compton scattering is taken into account.

Without Compton scattering: The temperature as a function of the Rosseland optical depth is given by a modification of the $T(\tau)$ relation for stellar atmospheres (Hubeny 1990), which in a simplified form that assumes the Eddington approximation reads

$$T^4 = \frac{3}{4}T_{\text{eff}}^4 \left[\tau \left(1 - \frac{\tau}{\tau_{\text{tot}}} \right) + \frac{1}{\sqrt{3}} + \frac{1}{3\epsilon\tau_{\text{tot}}} \frac{w}{\bar{w}} \right], \qquad (185)$$

where τ is the Rosseland optical depth, τ_{tot} is the τ at the central plane, and $\epsilon = \kappa_B/\kappa$, that is, the ratio of the Planck-mean to the Rosseland mean opacity. In a strict gray model, $\epsilon = 1$. If the total optical thickness of the disk is large, $\tau_{\text{tot}} \gg 1$, the last term in Eq. (185) is small.

With Compton scattering: The formalism is taken from Hubeny et al. (2001; their Eqs. (42-44). The local temperature is given by the solution of a fourth-order algebraic equation

$$\bar{\epsilon} \left(\frac{T}{T_{\text{eff}}} \right)^4 = \frac{3}{4} \left[\tau \left(1 - \frac{\tau}{2\tau_{\text{tot}}} \right) + \frac{1}{\sqrt{3}} \right] (\bar{\epsilon} - 2.867 \times 10^{-11} T) + \frac{1}{4\tau_{\text{tot}}} \frac{w}{\bar{w}}, \quad (186)$$

where

$$\bar{\epsilon} = \frac{\kappa_B}{n_e\sigma_{\text{T}}} \equiv \frac{\int_0^\infty \kappa_\nu B_\nu d\nu}{\int_0^\infty B_\nu d\nu} \frac{1}{n_e\sigma_{\text{T}}}. \qquad (187)$$

Equation (186) is solved by a Newton-Raphson method.

For each depth, starting with $d = 1$, the following iteration loop is performed: (*a*) first the increment of the Rosseland mean opacity is estimated (taken equal to the increment at the previous depth $d - 1$; the initial values at $d = 1$ are given by the input values); then the optical depth corresponding to depth d is determined.
(*b*) The temperature from Eq. (185) or (186) is calculated.
(*c*) Given the current values of T and P_g, one performs a $P_g \to \kappa$ procedure (that is, a part of the $P \to \kappa$ without its first step because we started already with the gas pressure).
(*d*) With the new value of κ one computes an updated optical depth τ and returns to step (*b*).
The loop (*b*) − (*d*) is repeated several times until the relative changes of T_d are sufficiently small.

3. Refinement of pressure, density, and vertical distance.

The values of the structural parameters are improved by a simultaneous solution of the hydrostatic equilibrium equation and the z-m relation. It turned out that a numerically more stable form of the hydrostatic equation is obtained by differentiating its original form, $dP/dm = Qz$ once more over m and using the exact expression $dz/dm = -1/\rho$, to obtain a second-order equation for P,

$$\frac{d^2P}{dm^2} = -\frac{Q}{\rho} = -\frac{Q}{c_s^2 P}, \qquad (188)$$

where the total sound speed $c_S = (P^{\mathrm{old}}/\rho^{\mathrm{old}})^{1/2}$ is taken as a known function of depth. The upper boundary condition is derived assuming that the temperature is constant for $m < m_1$, and integrating the hydrostatic equilibrium equation form depth m_1 upward. One obtains (Hubeny 1990)

$$m_1 = H_g \rho(z_1) f\left(\frac{z - H_r}{H_g}\right), \tag{189}$$

where

$$f(x) \equiv (\sqrt{\pi}/2) \exp(x^2)\, \mathrm{erfc}(x). \tag{190}$$

Here, H_g, H_r and c_S are evaluated using the current values of the state parameters at $d = 1$.

4. Changing the structure in the convection zone.

The procedure for changing temperature, and consequently the other state parameters, in the regions where the material is unstable against convection, is exactly the same as in the case of stellar atmospheres.

5   Conclusion

This document, which forms Part II of the three-paper series of a detailed user's guide for TLUSTY and SYNSPEC, contains an overview of physical assumptions, basic structural equations, and the description of the numerical methods to solve them. This paper thus provides a theoretical background for the next paper, which will provide a practical guide for working with TLUSTY. It will cover computational issues, namely a description of the input data and output files, a selection of appropriate options to fine-tune physical and numerical setup of the model construction, and basic troubleshooting.

Acknowledgements

Appendix A: Details of the formal solution of the transfer equation

As mentioned above, TLUSTY allows for several possibilities to perform a formal solution of the transfer equation. We recall that by the term *formal solution* we understand a solution with the thermal source function fully specified. If

the source function contains a scattering term, which is essentially always the case, this term is *not* assumed as given; instead it is treated self-consistently. The total number of depth points is ND; depth index d attains values between 1 (representing the uppermost point) and $d = ND$, representing the deepest point in the atmosphere. The angle points are labelled $i = 1, \ldots, NA$, with NA being the total number of angle points; their order is arbitrary.

We consider here the case where the transfer equation does not contain any coupling of the individual frequency points, and therefore it can be solved frequency by frequency. We thus skip an indication of the frequency dependence of the corresponding quantities, as well as the indices of discretized frequency points.

A1. Feautrier scheme

This is the standard method to solve the transfer equation with the known thermal source function. Here we also assume that the source function does not depend on angle.

The angle-dependent transfer equation is discretized as follows:

• for inner depth points, $d = 2, \ldots, ND - 1$,

$$\frac{\mu_i^2 j_{d-1,i}}{\Delta\tau_{d-1/2}\Delta\tau_d} - \frac{\mu_i^2 j_{di}}{\Delta\tau_d}\left(\frac{1}{\Delta\tau_{d-1/2}} + \frac{1}{\Delta\tau_{d+1/2}}\right) + \frac{\mu_i^2 j_{d+1,i}}{\Delta\tau_{d+1/2}\Delta\tau_d} = j_{di} - S_d, \quad (191)$$

where

$$\Delta\tau_d \equiv \frac{1}{2}(\Delta\tau_{d-1/2} + \Delta\tau_{d+1/2}), \tag{192}$$

The total source function is given by

$$S_d = \frac{\sigma_d}{\chi_d}\sum_{j=1}^{NA} w_{dj}j_{dj} + \frac{\eta_d}{\chi_d}. \tag{193}$$

• upper boundary condition, in the second-order form, is given by

$$\mu_l\frac{j_{2i} - j_{1i}}{\Delta\tau_{3/2}} = j_{1i} - I_i^{\text{ext}} + \frac{\Delta\tau_{3/2}}{2\mu_i}(j_{1i} - S_{1l}) \tag{194}$$

• For the lower boundary, $d = ND$, there are two possible forms, one for stellar atmospheres, with diffusion approximation, and one for accretion disks, with symmetry boundary condition, $dj/d\tau|_{ND} = 0$. Both are considered in the second-order form.

  – For stellar atmospheres

$$\mu_i\frac{j_{di} - j_{d-1,i}}{\Delta\tau_{d-1/2}} = I_i^+ - j_{di} - \frac{\Delta\tau_{d-1/2}}{2\mu_i}(j_{di} - S_d), \tag{195}$$

where

$$I_i^+ = B_{ND} + \mu_i\frac{B_{ND} - B_{ND-1}}{\Delta\tau_{ND-1/2}}. \tag{196}$$

– For accretion disks

$$\mu_i \frac{j_{di} - j_{d-1,i}}{\Delta\tau_{d-1/2}} = -\frac{\Delta\tau_{d-1/2}}{2\mu_i}(j_{di} - S_d), \tag{197}$$

One introduces a column vector $\mathbf{j}_d \equiv \{j_{d1}, j_{d2}, \ldots, j_{d,NA}\}^T$, and the set of equations (191), (193) - (196) is expressed as a block tridiagonal system of the form

$$-\mathbf{A}_d\,\mathbf{j}_{d-1} + \mathbf{B}_d\,\mathbf{j}_d - \mathbf{C}_d\,\mathbf{j}_{d+1} = \mathbf{R}_d \quad (d = 1, \ldots, ND). \tag{198}$$

$\mathbf{A}_d$, $\mathbf{B}_d$, and $\mathbf{C}_d$ are ($NA \times NA$) matrices. $\mathbf{A}_d$ and $\mathbf{C}_d$ are diagonal, containing the finite–difference terms in (191) that couple the angle–frequency components of $\mathbf{j}_{di}$ at depth point d to those at depth points $d-1$ and $d+1$ respectively. $\mathbf{R}_d$ is a column vector of length NA, containing the thermal (i.e. non–scattering) source terms in (193).

At an interior point ($d = 2$, ..., $ND - 1$), ($i, j = 1$, ..., NA),

$$(\mathbf{A}_d)_{ij} = \mu_i^2/(\Delta\tau_{d-1/2}\,\Delta\tau_d)\,\delta_{ij}, \tag{199}$$

$$(\mathbf{C}_d)_{ij} = \mu_i^2/(\Delta\tau_{d+1/2}\,\Delta\tau_d)\,\delta_{ij}, \tag{200}$$

$$(\mathbf{B}_d)_{ij} = \delta_{ij} + (\mathbf{A}_d)_{ij} + (\mathbf{C}_d)_{ij} - (\sigma_d/\chi_d)w_j, \tag{201}$$

$$(\mathbf{R}_d)_i = \eta_d/\chi_d. \tag{202}$$

Here δ_{ij} is the Kronecker symbol.

At the upper boundary, $d = 1$, one has $(\mathbf{A}_1)_{ij} \equiv 0$, and

$$(\mathbf{B}_d)_{ij} = [1 + (2\mu_i/\Delta\tau_{d+1/2}) + 2(\mu_i/\Delta\tau_{d+1/2})^2]\,\delta_{ij} - (\sigma_d/\chi_d)w_j, \tag{203}$$

$$(\mathbf{C}_d)_{ij} = 2(\mu_i/\Delta\tau_{d+1/2})^2\,\delta_{ij}, \tag{204}$$

and

$$\mathbf{R}_{di} = \eta_d/\chi_d + (2\mu_i/\Delta\tau_{d+1/2})I_i^{\text{ext}}. \tag{205}$$

For the lower boundary, $d = ND$, one has $(\mathbf{C}_{ND})_{ij} = 0$, and
– for stellar atmospheres

$$(\mathbf{B}_d)_{ij} = [1 + (2\mu_i/\Delta\tau_{d-1/2}) + 2(\mu_i/\Delta\tau_{d-1/2})^2]\delta_{ij} - (\sigma_d/\chi_d)\,w_j, \tag{206}$$

$$(\mathbf{A}_d)_{ij} = 2(\mu_i/\Delta\tau_{d-1/2})^2\,\delta_{ij}, \tag{207}$$

$$(\mathbf{R}_d)_i = \sigma_d/\chi_d - (2\mu_i/\Delta\tau_{d-1/2})I_{d,i}^+. \tag{208}$$

– for accretion disks

$$(\mathbf{B}_d)_{ij} = [1 + 2(\mu_i/\Delta\tau_{d-1/2})^2]\,\delta_{ij} - (\sigma_d/\chi_d)\,w_j, \tag{209}$$

$$(\mathbf{A}_d)_{ij} = 2(\mu_i/\Delta\tau_{d-1/2})^2\,\delta_{ij}, \tag{210}$$

and

$$(\mathbf{R}_d)_i = \sigma_d/\chi_d, \tag{211}$$

Equation (198) is solved by a standard Gauss-Jordan elimination that consists of a forward elimination, analogously to that employed for complete linearization, Eqs, (123) - (125),

$$\mathbf{D}_1 = \mathbf{B}_1^{-1}\mathbf{C}_1, \quad \text{and} \quad \mathbf{D}_d = (\mathbf{B}_d - \mathbf{A}_d\mathbf{D}_{d-1})^{-1}\mathbf{C}_d, \quad d = 2, \ldots, ND, \quad (212)$$

and

$$\mathbf{Z}_1 = \mathbf{B}_1^{-1}\mathbf{L}_1, \quad \text{and} \quad \mathbf{Z}_d = (\mathbf{B}_d - \mathbf{A}_d\mathbf{D}_{d-1})^{-1}(\mathbf{L}_d + \mathbf{A}_d\mathbf{Z}_{d-1}), \quad d = 2, \ldots, N. \quad (213)$$

followed by a back-substitution

$$\delta\psi_{ND} = \mathbf{Z}_{ND}, \quad \text{and} \quad \delta\psi_d = \mathbf{D}_d\delta\psi_{d+1} + \mathbf{Z}_d, \quad d = ND - 1, \ldots, 1. \quad (214)$$

Scalar Feautrier scheme

Once the solution for $\mathbf{j}$ is obtained by the procedure described by Eqs. (212) - (214), the mean intensity and the Eddington factors are computed using (156). This procedure may be sufficient. However, for the overall consistency, the transfer equation needs to be solved again, now for the mean intensity using the newly determined Eddington factors. The reason for this is that such an equation is being considered as one of the structural equations. Although its solution for the mean intensity is mathematically equivalent to the corresponding integral of the solution of the angle-dependent transfer equation, these solutions are slightly different numerically due to rounding errors, and due to inaccuracies in numerical integration over angles. One should therefore enter the next linearization step with a current solution of the same equation that is linearized; otherwise the global iteration process would stop converging at small but non-zero relative changes.

The discretized combined moment equation is written as follows:
• For inner depth points, $d = 2, \ldots, ND - 1$, one has

$$\frac{f_{d-1}J_{d-1}}{\Delta\tau_{d-1/2}\Delta\tau_d} - \frac{f_dJ_d}{\Delta\tau_d}\left(\frac{1}{\Delta\tau_{d-1/2}} + \frac{1}{\Delta\tau_{d+1/2}}\right) + \frac{f_{d+1}J_{d+1}}{\Delta\tau_{d+1/2}\Delta\tau_d} = J_d - S_d. \quad (215)$$

The right–hand side of equation (215) can be written as

$$J_d - S_d = \epsilon_dJ_d - \frac{\eta_d}{\chi_d}, \quad (216)$$

with

$$\epsilon_d \equiv 1 - \sigma_d/\chi_d = \kappa_d/\chi_d. \quad (217)$$

• The upper boundary condition ($d = 1$), in the second–order form that follows from integrating equation (194) over angles, is

$$\frac{f_{d+1}J_{d+1} - f_dJ_d}{\Delta\tau_{d+1/2}} = gJ_d - H^{\text{ext}} + \frac{\Delta\tau_{d+1/2}}{2}\left(\epsilon_dJ_d - \frac{\eta_d}{\chi_d}\right). \quad (218)$$

• The lower boundary condition ($d = ND$) is again different for semi-infinite atmospheres and for accretion disks.

  – For stellar atmospheres, assuming the diffusion approximation,

$$\frac{f_s J_s - f_{d-1} J_{d-1}}{\Delta \tau_{d-1/2}} = \frac{1}{2}(\mathcal{B}_d - J_d) + \frac{\mathcal{B}_d - \mathcal{B}_{d-1}}{3 \Delta \tau_{d-1/2}} - \frac{\Delta \tau_{d-1/2}}{2}\left(\epsilon_d J_d - \frac{\eta_d}{\chi_d}\right), \quad (219)$$

where $\mathcal{B}$ denotes the Planck function.

  – For accretion disks, one also employs a second-order form in which one uses the symmetry condition $(dj/d\tau)_{ND} = 0$,

$$\frac{2}{\Delta \tau_{d-1/2}} \frac{f_d J_d - f_{d-1} J_{d-1}}{\Delta \tau_{d-1/2}} + \epsilon_d = \frac{\eta_d}{\chi_d}. \quad (220)$$

Equations (215), (218), and (219) also form a tridiagonal system

$$-A_d J_{d-1} + B_d J_d - C_d J_{d+1} = R_d, \quad (221)$$

where now A_d, B_d, and C_d are scalars (real numbers). They are given by

$$A_d = \begin{cases} 0, & \text{for } d = 1, \\ f_{d-1}/[\Delta \tau_{d-1/2} \Delta \tau_d], & \text{for } d \geq 2, \end{cases} \quad (222)$$

$$B_d = \begin{cases} (f_d/\Delta \tau_{d+1/2}) + g + \epsilon \Delta \tau_{d+1/2}/2, & d = 1, \\ (f_d/\Delta \tau_d)\left[\Delta \tau_{d-1/2}^{-1} + \Delta \tau_{d+1/2}^{-1}\right] + \epsilon, & d = 2, \ldots, ND-1, \\ (f_d/\Delta \tau_{d-1/2}) + (1/2) + \epsilon \Delta \tau_{d-1/2}/2, & d = ND, \end{cases} \quad (223)$$

$$C_d = \begin{cases} f_{d+1}/[\Delta \tau_{d+1/2} \Delta \tau_d], & d < ND, \\ 0 & d = ND, \end{cases} \quad (224)$$

and

$$R_d = \begin{cases} H^{\text{ext}} + (\Delta \tau_{d+1/2}/2)(\eta_d/\chi_d), & d = 1, \\ (\eta_d/\chi_d), & d = 2, \ldots, ND-1, \\ X^+ - \epsilon \Delta \tau_{d-1/2}/2, & d = ND, \end{cases} \quad (225)$$

where

$$X^+ = \mathcal{B}_{ND}/2 + (\mathcal{B}_{ND} - \mathcal{B}_{ND-1})/(3 \Delta \tau_{ND-1/2}) \quad (226)$$

Equation (221) is solved analogously as described above.

A2. Fourth-order Hermitian scheme

This efficient and very accurate modification of the standard Feautrier scheme was suggested by Auer (1976). The finite difference scheme originally expressed by Eq. (191) is replaced by

$$-A_d\, j_{d-1} + B_d\, j_d - C_d\, j_{d+1} + \alpha_d\, j''_{d-1} + \beta_d\, j''_d + \gamma_d\, j''_{d+1} = 0, \quad (227)$$

where $j_d'' \equiv \mu^2 \, d^2 j/d\tau^2|_d = j_d - S_d$. Expanding $j_{d\pm1}$ and $j_{d\pm1}''$ to fourth order Taylor series, one obtains after some algebra (see Auer 1967; or Hubeny & Mihalas 2014, $\S$12.4) a block-tridiagonal system analogous to the standard Feautrier scheme, Eq. (198), where now

$$(\mathbf{A}_d)_{ij} = (a_{di} - \alpha_{di})\delta_{ij} + \alpha_{di}\,(\sigma_{d-1}/\chi_{d-1})\,w_j, \tag{228}$$

$$(\mathbf{C}_d)_{ij} = (c_{di} - \gamma_{di})\delta_{ij} + \gamma_{di}(\sigma_{d+1}/\chi_{d+1})\,w_j, \tag{229}$$

$$(\mathbf{B}_d)_{ij} = (b_{di} + \beta_{di})\delta_{ij} - \beta_{di}(\sigma_d/\chi_d)\,w_j, \tag{230}$$

and

$$\mathbf{R}_{di} = \alpha_{di}(\eta_{d-1}/\chi_{d-1}) + \beta_{di}(\eta_d/\chi_d) + \gamma_{di}(\eta_{d+1}/\chi_{d+1}), \tag{231}$$

where the individual auxiliary quantities are given by

$$a_{di} = \mu_i^2/(\Delta\tau_d\Delta\tau_{d-1/2}), \tag{232}$$

$$c_{di} = \mu_i^2/(\Delta\tau_d\Delta\tau_{d+1/2}), \tag{233}$$

$$b_{di} = a_{di} + c_{di}, \tag{234}$$

$$\alpha_{di} = [1 - a_{di}\Delta\tau_{d+1/2}^2/(2\mu_i^2)]/6, \tag{235}$$

$$\gamma_{di} = [1 - c_{di}\Delta\tau_{d-1/2}^2/(2\mu_i^2)]/6, \tag{236}$$

$$\beta_{di} = 1 - \alpha_{di} - \gamma_{di}, \tag{237}$$

Although one can construct a third-order form for the boundary condition, the usual second-order form expressed by Eqs. (203) - (211) is satisfactory, and is being used in TLUSTY.

A3. Improved Rybicki-Hummer solution algorithm

In this variant of the Feautrier scheme, the basic expressions Eq. (191) - (197) remain unchanged, the only point which is changed is the method of the solution of the resulting tri-diagonal system (198). It can obviously be used in conjunction with the 4-th order Hermitian scheme as well.

This scheme has better numerical properties if $\Delta\tau \ll 1$, which may easily happen near the surface. In this case, the terms proportional to $\Delta\tau^{-2}$ are very large, which cause the other terms ("1" from the Kronecker δ, and the term corresponding to scattering source function term), may be lost because of a limited numerical representation, or be inaccurate due to numerical noise. In this case, one changes the original algorithm by introducing an auxiliary quantity

$$H_d = -A_d + B_d - C_d, \tag{238}$$

(with $A_1 = C_{ND} = 0$), and

$$F_d = D_d^{-1} - 1. \tag{239}$$

and the solution algorithm, originally described by Eqs. (123) - (125), proceeds now as follows

$$F_d = C_d^{-1}\{H_d + A_d \cdot [1 - (1 + F_{d-1})^{-1}]\}, \qquad (240)$$

$$E_d = (1 + F_d)^{-1}C_d^{-1}(R_d + A_dE_{d-1}), \qquad (241)$$

The reverse sweep starts with $j_{ND} = E_{ND}$, followed by for $d = ND - 1, \ldots, 1$,

$$j_d = (1 + F_d)^{-1}j_{d+1} + E_d. \qquad (242)$$

This formalism applies both for the block-tridiagonal systems of equations (198), in which case A, B, C, H, D, F, and E are matrixes, as well as by Eq. (221), in which case they are scalars.

A4. Discontinuous Finite Elements

If an atmospheric structure exhibits very sharp variations with depth, it is advantageous to use the Discontinuous Finite Element (DFE) scheme by Castor et al. (1992). It solves the linear transfer equation

$$\frac{dI_\nu}{d\widetilde{\tau}_\nu} = I_\nu - S_\nu, \qquad (243)$$

where $\widetilde{\tau}_\nu \equiv \tau_\nu/|\mu|$ is the optical depth along the line of propagation of radiation. Equation (243) is solved directly for the specific intensity, and therefore the scattering part of the source function has to be treated iteratively. To this end, a simple ALI-based procedure is used. It is outlined below. Here we describe the method assuming that the total source function is fully specified.

The method is essentially an application of the Galerkin method. An idea is to divide a medium into a set of cells, and to represent the source function within a cell by a simple polynomial, in this case by a linear segment. The crucial point is that the segments are assumed to have step discontinuities at grid points. The specific intensity at grid point d is thus characterized by two values I_d^+ and I_d^- appropriate for cells $(\widetilde{\tau}_d, \widetilde{\tau}_{d+1})$ and $(\widetilde{\tau}_{d-1}, \widetilde{\tau}_d)$, respectively. Notice that we are dealing with an intensity in a given direction; the superscripts "+" and "−" thus do not denote intensities in opposite directions as it is usually used in the radiative transfer theory. The actual value of the specific intensity $I(\widetilde{\tau}_d)$ is given as an appropriate linear combination of I_d^+ and I_d^-. We skip all details here; suffice to say that after some algebra one obtains simple recurrence relations for I_d^+ and I_d^-, for $d = 1, \ldots, ND - 1$,

$$a_dI_{d+1}^- = 2I_d^- + \Delta\widetilde{\tau}_{d+1/2}S_d + b_dS_{d+1}, \qquad (244)$$

$$a_dI_d^+ = 2(\Delta\widetilde{\tau}_{d+1/2} + 1)I_d^- + b_dS_d - \Delta\widetilde{\tau}_{d+1/2}S_{d+1}, \qquad (245)$$

where

$$a_d = \Delta\widetilde{\tau}_{d+1/2}^2 + 2\Delta\widetilde{\tau}_{d+1/2} + 2, \qquad (246)$$

$$b_d = \Delta\widetilde{\tau}_{d+1/2}(\Delta\widetilde{\tau}_{d+1/2} + 1), \qquad (247)$$

and

$$\Delta\widetilde{\tau}_{d+1/2} = \widetilde{\tau}_{d+1} - \widetilde{\tau}_d, \tag{248}$$

The boundary condition is $I_1^- = I^{\mathrm{ext}}$, where I^{ext} is the specific intensity of external irradiation (for inward-directed rays, $\mu < 0$).

For outward-directed rays ($\mu > 0$), one can either use the same expressions as above, renumbering the depth points such as $ND \to 1, ND{-}1 \to 2, \dots, 1 \to ND$; or use the same numbering of depth points while setting the recursion, for $d = ND - 1, \dots, 1$, as

$$a_d I_d^- = 2I_{d+1}^- + \Delta\widetilde{\tau}_{d+1/2} S_{d+1} + b_d S_d, \tag{249}$$

$$a_d I_{d+1}^+ = 2(\Delta\widetilde{\tau}_{d+1/2} + 1)\, I_{d+1}^- + b_d S_{d+1} - \Delta\widetilde{\tau}_{d+1/2} S_d, \tag{250}$$

with $I_d^- = B_d + \mu(B_d - B_{d-1})/\Delta\widetilde{\tau}_{d-1/2}$, i.e., assuming the diffusion approximation, for $d = ND$.

Finally, the resulting specific intensity at $\widetilde{\tau}_d$ is given by a linear combination of the "discontinuous" intensities I_d^- and I_d^+ as

$$I_d = \frac{I_d^- \Delta\widetilde{\tau}_{d+1/2} + I_d^+ \Delta\widetilde{\tau}_{d-1/2}}{\Delta\widetilde{\tau}_{d+1/2} + \Delta\widetilde{\tau}_{d-1/2}}. \tag{251}$$

At the boundary points, $d = 1$ and $d = ND$, we set $I_d = I_d^-$. As was shown by Castor et al. (1992), it is exactly the linear combination of the discontinuous intensities expressed in Eq. (251) which makes the method second-order accurate. Since one does not need to evaluate any exponentials, the method is also very fast.

We stress again that the above scheme applies for a solution of the transfer equation along a single line of sight; that is, for a single angle of propagation. The source function is assumed to be given. Therefore, when scattering is not negligible, one has to iterate on the source function. This is done using an application of the Accelerated Lambda Iteration (ALI) method.

Here is an algorithm to use the ALI scheme in this context, assuming a diagonal Λ^* operator. For more details refer to Hubeny & Mihalas (2014, § 13.5):

(i) For a given S^{old} (with an initial estimate $S^{\mathrm{old}} = B$ or some other suitable value), perform a formal solution of the transfer equation, one frequency and direction (given μ) at a time. This yields a new value of the specific intensity I_μ and also the values of the Λ_μ^*, angle-dependent approximate operator – see below.

(ii) By integrating over directions using

$$J^{\mathrm{FS}} = \frac{1}{2} \int_{-1}^{1} d\mu\, \Lambda_\mu[S^{\mathrm{old}}] \tag{252}$$

obtain new values of the formal-solution mean intensity J^{FS}. Here, the action of the Λ operator simply means obtaining the specific intensity by

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solving the transfer equation using the old source function. Analogously, compute the angle-integrated $\bar{\Lambda}^*$ as

$$\bar{\Lambda}^* = \frac{1}{2} \int_{-1}^{1} d\mu \, \Lambda_\mu^*, \tag{253}$$

(iii) Evaluate a new iterate of the mean intensity as $J^{\mathrm{new}} = J^{\mathrm{old}} + \delta J$, where

$$\delta J = \frac{J^{\mathrm{FS}} - J^{\mathrm{old}}}{1 - (1 - \epsilon)\bar{\Lambda}^*}. \tag{254}$$

(iv) If the mean intensity found in step (iii) differs from that used in step (i), update the source function from (193) using the newly found mean intensity and repeat steps (i) to (iii) to convergence.

A5. Construction of the approximate Λ^* operator

As mentioned above, one has to construct the approximate Λ^* operator in the formal solution of the transfer equation. This operator is then held fixed during the subsequent step of the linearization procedure.

As explained in Hubeny & Mihalas (2014; § 13.3), the matrix elements of the Λ operator can be evaluated by setting the source function to be the unit pulse function, $S(\tau_d) = \delta(\tau - \tau_d)$, so that

$$\Lambda_{dd'} = \Lambda_{\tau_d}[\delta(\tau_{d'} - \tau)], \tag{255}$$

In practice, one does not have to solve the full transfer equation, but only to collect coefficients that stand at S_d in the expressions to evaluate I_d. The actual evaluation depends on the type of the formal solver of the transfer equation

Using the Feautrier scheme

The procedure, following Rybicki & Hummer (1991), is as follows. Let $\mathbf{T}$ be an $N \times N$ tridiagonal matrix and let its inverse be $\Lambda \equiv \mathbf{T}^{-1}$. The equation for the inverse can be written as $\mathbf{T} \cdot \mathbf{\Lambda} = \mathbf{1}$, or, in component form

$$-A_i \lambda_{i-1,j} + B_i \lambda_{ij} - C_i \lambda_{i+1,j} = \delta_{ij}. \tag{256}$$

For any fixed value of j this equation can be solved by one of the forms of Gaussian elimination. In the usual implementation the elimination proceeds from $i = 1$ to $i = N$, followed by back–substitution from $i = N$ to $i = 1$,

$$D_i = (B_i - A_i D_{i-1})^{-1} C_i, \tag{257}$$

$$Z_{ij} = (B_i - A_i D_{i-1})^{-1}(\delta_{ij} + A_i Z_{i-1,j}), \tag{258}$$

and

$$\lambda_{ij} = D_i \lambda_{i+1,j} + Z_{ij}. \tag{259}$$

It is also possible to implement the method in reverse order,

$$E_i = (B_i - C_i E_{i+1})^{-1} A_i, \tag{260}$$

$$W_{ij} = (B_i - C_i E_{i+1})^{-1}(\delta_{ij} + C_i W_{i+1,j}), \tag{261}$$

and

$$\lambda_{ij} = E_i \lambda_{i-1,j} + W_{ij}. \tag{262}$$

The crucial idea of the method is to use parts of *both* of these implementations to find the diagonal elements λ_{ii}.

Since $\delta_{ij} = 0$ for $i \neq j$, it follows from (258) and (261) that $Z_{ij} = 0$ for $i < j$, and $W_{ij} = 0$ for $i > j$. Thus, from (258) and (259) we obtain, for special choices of i and j,

$$Z_{ii} = (B_i - A_i D_{i-1})^{-1}, \tag{263}$$

$$\lambda_{ii} = D_i \lambda_{i+1,i} + Z_{ii}, \tag{264}$$

$$\lambda_{i-1,i} = D_{i-1} \lambda_{ii}, \tag{265}$$

and, from (261) and (262)

$$W_{ii} = (B_i - C_i E_{i+1})^{-1}, \tag{266}$$

$$\lambda_{ii} = E_i \lambda_{i-1,i} + W_{ii}, \tag{267}$$

and

$$\lambda_{i+1,i} = E_{i+1} \lambda_{ii}. \tag{268}$$

Using (263), (264), and (268) we eliminate Z_{ii} and $\lambda_{i+1,i}$ to obtain

$$\lambda_{ii} = (1 - D_i E_{i+1})^{-1}(B_i - A_i D_{i-1})^{-1}. \tag{269}$$

The right hand side now depends only on the single–indexed quantities A_i and B_i, which are given, and D_i and E_i which can be found by two passes through the depth grid, using the recursion relations (257) and (260). Thus λ_{ii} can be found in order N operations.

An evaluation of the approximate operator requires only little extra work in the formal solution. The quantities A_i, B_i, C_i, and D_i are common to both problems, and one needs only to include the recursion relation (260) as part of the back–substitution to find the auxiliary quantities E_i.

Using the Discontinuous Finite element method

When using the DFE scheme for the formal solution of the transfer equation, one proceeds along the recurrence relations (244) and (245) to compute

$$L_{d+1}^- = b_d/a_d, \tag{270}$$

$$L_d^+ = [2(\Delta\tilde{\tau}_{d+1/2} + 1) L_d^- + b_d]/a_d \tag{271}$$

where a_d and b_d are given by (246) and (247). The complete diagonal element of the (angle-dependent) elementary operator is obtained, in parallel with Eq. (251), as

$$\Lambda_d^*(\mu, \phi) \equiv \Lambda_{dd} = \frac{L_d^- \Delta\widetilde{\tau}_{d+1/2} + L_d^+ \Delta\widetilde{\tau}_{d-1/2}}{\Delta\widetilde{\tau}_{d+1/2} + \Delta\widetilde{\tau}_{d-1/2}}. \tag{272}$$

The values at the boundaries are $\Lambda_{dd} = 0$ for $d = 1$, and $\Lambda_{dd} = L_d^-$ for $d = ND$. The evaluation of the diagonal elements for outward-directed rays is analogous,

$$L_d^- = b_d/a_d, \tag{273}$$
$$L_{d+1}^+ = [2(\Delta\widetilde{\tau}_{d+1/2} + 1) L_{d+1}^- + b_d]/a_d \tag{274}$$

As stressed above, the solution of the transfer equation using the DFE method is performed for one direction at a time, so L and Λ in Eqs. (270) - (272) are also specified for given μ and ϕ. The total approximate operator needed to evaluate the new iterate of the source function or the mean intensity is given by

$$\bar{\Lambda}_d^* = \frac{1}{4\pi} \int_0^{2\pi} d\phi \int_{-1}^1 d\mu \, \Lambda_d^*(\mu, \phi). \tag{275}$$

A6. Compton scattering

The basic complication in the formal solution is that one can no longer solve the transfer equation frequency by frequency independently, as it is done in the standard treatment, but the coupling of frequencies expressed by Eq. (93) has to be taken into account. Although one can devise an ALI-based method that would be efficient and universal, this is not yet done in TLUSTY, where one resorts to the direct scheme.

Such a scheme was developed by Hubeny et al. (2001); here we point out only the basic features. The angle-averaged Compton scattering source function is given by

$$S_\nu^{\text{Compt}} = (1 - x)J_\nu + (x - 3\Theta)J_\nu' + \Theta J_\nu'' + \frac{c^2}{2h\nu^3} J_\nu 2x(J_\nu' - J_\nu), \tag{276}$$

where

$$x = \frac{h\nu}{m_{\text{e}}c^2}, \quad \Theta = \frac{kT}{m_{\text{e}}c^2}, \tag{277}$$

The second-order form of the radiative transfer equation, discretized in frequency, is written for the i-th frequency point as [see Hubeny et al. (2001), eq. (A51)],

$$\frac{\partial^2(f_i J_i)}{\partial \tau_i^2} = J_i - \epsilon_i S_i^{\text{th}} - (\mathcal{A}_i J_{i-1} + \mathcal{B}_i J_i + \mathcal{C}_i J_{i+1}) + J_i(\mathcal{U}_i J_{i-1} + \mathcal{E}_i J_i + \mathcal{V}_i J_{i+1}), \tag{278}$$

where $\epsilon_i = \kappa_i^{\text{th}}/(\kappa_i^{\text{th}} + \sigma_i)$, $\lambda_i = 1 - \epsilon_i$. Here, and in the following, we skip the depth index d.

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Since Eq. (278) represents a discretized version of a partial differential equation in depth and frequency, one need to invoke specific initial conditions of the lowest and highest frequency.

We will first consider the internal frequency points, $\nu_i, 2 \leq i \leq NF - 1$. The coefficients $\mathcal{A}, \mathcal{B}, \mathcal{C}, \mathcal{E}, \mathcal{U}, \mathcal{V}$ are expressed by two possible ways. The original approach is that developed in Hubeny et al. (2001), viz.

$$
\begin{align}
\mathcal{A}_i &= \lambda_i[(x_i - 3\Theta)c_i^- + \Theta d_i^-], & (279)\\
\mathcal{B}_i &= \lambda_i[(1 - x_i) + (x_i - 3\Theta)c_i^0 + \Theta d_i^0], & (280)\\
\mathcal{C}_i &= \lambda_i[(x_i - 3\Theta)c_i^+ + \Theta d_i^+], & (281)\\
\mathcal{E}_i &= \lambda_i[(2h\nu_i^3/c^2)2x_i(c_i^0 - 1)], & (282)\\
\mathcal{U}_i &= \lambda_i(2h\nu_i^3/c^2)2x_ic_i^-, & (283)\\
\mathcal{V}_i &= \lambda_i(2h\nu_i^3/c^2)2x_ic_i^+. & (284)
\end{align}
$$

There is another, preferable approach, based on the formalism of Chang & Cooper (1970), where,

$$
\begin{align}
\mathcal{A}_i &= \lambda_i[-\delta_{i-1}y_{i-1} + \Theta d_i^-], & (285)\\
\mathcal{B}_i &= \lambda_i[\delta_i y_{i+1} + (1 - \delta_{i-1})y_{i-1} + \Theta d_i^0 - \epsilon_i + 1, & (286)\\
\mathcal{C}_i &= \lambda_i[(1 - \delta_i)y_{i+1} + \Theta d_i^+], & (287)\\
\mathcal{E}_i &= \mathcal{U}_i = \mathcal{V}_i = 0, & (288)
\end{align}
$$

where

$$
\begin{align}
y_i &= [(1 - \delta_i)z_{i+1} + \delta_i z_i]\Delta_0, & (289)\\
z_i &= x_i[1 + J_i c^2/(2h\nu_i^3)] - 3\Theta. & (290)
\end{align}
$$

In Eq. (290) , one takes for J_i the current, and thus known, specific intensity. This avoids a non-linearity of the transfer equation that would arise due to stimulated emission.

In both cases, the coefficients c_i^0, c_i^-, and c_i^+ come from discretizing the first derivative terms in Eq. (276),

$$
\begin{align}
c_i^+ &= (1 - \delta_i)/\Delta_i, \quad c_i^- = -\delta_{i-1}/\Delta_i, & (291)\\
c_i^0 &= -c_i^+ - c_i^-, & (292)
\end{align}
$$

where

$$
\begin{align}
\Delta_{i-1/2} &= \ln(\nu_i/\nu_{i-1}), \quad \Delta_{i+1/2} = \ln(\nu_{i+1}/\nu_i), & (293)\\
\Delta_i &= \Delta_{i-1/2} + \Delta_{i+1/2}. & (294)
\end{align}
$$

The coefficients δ_i are determined by solving a quadratic equation

$$
a\,\delta_i^2 + b\,\delta_i + c = 0, \tag{295}
$$

where the coefficients a, b, c are given by, using the original approach (Hubeny et al. 2011) as

$$a = \Delta B_i \, \delta \beta_i, \tag{296}$$
$$b = \Delta B_i \, (1 + \beta_{i+1} - 3/\bar{\xi}) + B_{i+1} \, \delta \beta_i, \tag{297}$$
$$c = B_{i+1}(1 + \beta_{i+1} - 3/\bar{\xi}) - \Delta B_i / [\bar{\xi} \ln(\nu_{i+1}/\nu_i)], \tag{298}$$

where $\bar{\xi} = (h/kT)(\nu_i \nu_{i+1})^{1/2}$; or, using the Chang & Cooper (1970) approach, as

$$a = \Delta B_i \, \delta z_i, \tag{299}$$
$$b = \Delta B_i \, z_{i+1} + B_{i+1} \, \delta z_i, \tag{300}$$
$$c = B_{i+1} z_{i+1} - \Theta \, \Delta B_i / \Delta_i \tag{301}$$

where, in both cases,

$$z_i = x_i(1 + \beta_i) - 3\Theta, \quad \Delta z_i = z_i - z_{i+1}, \tag{302}$$
$$\beta_i = [\exp(h\nu_i/kT) - 1]^{-1}, \tag{303}$$
$$B_i = (2h\nu_i^3/c^2)\beta_i, \quad \Delta B_i = B_i - B_{i+1}. \tag{304}$$

In both cases, one picks the solution of (295) which satisfies $0 \le \delta_i \le 1/2$.

The analogous coefficients d_i come from the second derivative terms.

$$d_i^- = 2(\Delta_{i-1/2}\Delta_i)^{-1}, \quad d_i^+ = 2(\Delta_{i+1/2}\Delta_i)^{-1}, \tag{305}$$
$$d_i^0 = -d_i^+ - d_i^-. \tag{306}$$

The non-linear terms in Eq. (276), corresponding to the stimulated emission, are linearized by using the "old" intensities, replacing B_i by B_i', where

$$\mathcal{B}_i' = \mathcal{B}_i + \mathcal{U}_i J_{i-1}^{\text{old}} + \mathcal{E}_i J_i^{\text{old}} + \mathcal{V}_i J_{i+1}^{\text{old}}. \tag{307}$$

In the case of the Chang & Cooper approach, the stimulated emission terms were already included, as is seen in Eq. (290), so $\mathcal{B}_i' = \mathcal{B}_i$.

The initial condition for the lowest frequency, $i = 1$, which is assumed to be very low, is simply

$$\mathcal{B}_i = 1 - 2x_i, \tag{308}$$

and all the other coefficients $\mathcal{A}_i = \mathcal{C}_i = \mathcal{E}_i = \mathcal{U}_i = \mathcal{V}_i = 0$.

The initial condition for the highest frequency, $i = NF$, is more complicated. In the original approach after Hubeny et al. (2001) one has

$$\mathcal{A}_i = -\xi_0 / \ln(\nu_i/\nu_{i-1}) + (1 - \delta_{i-1})\xi_1, \tag{309}$$
$$\mathcal{B}_i = \xi_0 / \ln(\nu_i/\nu_{i-1}) + \delta_{i-1}\xi_1, \tag{310}$$

where

$$\xi_0 = kT/[h(\nu_i \nu_{i-1})^{1/2}], \tag{311}$$
$$\xi_1 = 1 - 3\xi_0 + (1 - \delta_{i-1})e^{-h\nu_i/kT} + \delta_{i-1}e^{-h\nu_{i-1}/kT}, \tag{312}$$

In the case of Chang & Cooper approach, one has

$$\mathcal{A}_i = -\Theta/\delta_{i-1} + (1 - \delta_{i-1})\zeta_0, \tag{313}$$

$$\mathcal{B}_i = \Theta/\delta_{i-1} + \delta_{i-1}\zeta_0, \tag{314}$$

where

$$\zeta_0 = (1 - \delta_{i-1})\zeta_i + \delta_{i-1}\zeta_{i-1}, \tag{315}$$

$$\zeta_i = x_i \left(1 + e^{-h\nu_i/kT}\right) - 3\Theta. \tag{316}$$

The left-hand side of Eq. (278) is discretized as in the ordinary transfer problem, so that the final algebraic equation for the mean intensities reads

$$-\alpha_{id}J_{i,d-1} - \gamma_{id}J_{i,d+1} + (\beta_{id} + 1 - \mathcal{B}'_{id})J_{id} - \mathcal{A}_{id}J_{i-1,d} - \mathcal{C}_{id}J_{i+1,d} = \epsilon_{id}S_{id}^{\rm th}. \tag{317}$$

One can use equation (317) in two different ways, called in vague analogy with the hydrodynamical terminology as *explicit* or *implicit*.

(i) The **implicit** way consists of solving Eq. (317) with the full coupling taken into account; that is, all the mean intensities, including those in frequency points $i - 1$ and $i + 1$, are solved for. This approach is more stable, but it involves a more time-consuming solution of the coupled problem. It is solved by a standard scheme. One introduces a column vector $\mathbf{J}_i \equiv (J_{i1}, J_{i2}, \ldots, J_{iD})$, where $D \equiv ND$ being the number of depth points, and write Eq. (317) as a linear matrix equation

$$-\mathbf{A}_i\mathbf{J}_{i-1} + \mathbf{B}_i\mathbf{J}_i - \mathbf{C}_i\mathbf{J}_{i+1} = \mathbf{L}_i, \tag{318}$$

where the elements of the matrices are given by the corresponding coefficients $\mathcal{A}_{id}$, $\mathcal{B}'_{id}$, $\mathcal{C}_{id}$, α_{id}, β_{id}, and γ_{id}, and vector $(\mathbf{L}_i) = \epsilon_{id}S_{id}^{\rm th}$. Matrices $\mathbf{B}$ are tridiagonal (because of a difference representation of the second derivative with respect to depth), and matrices $\mathbf{A}$ and $\mathbf{C}$ are diagonal (because the terms containing the frequency derivatives are local). Equation (318) is solved by a standard Gauss-Jordan elimination.

(ii) The **explicit** way consists of avoiding the frequency coupling by considering the radiation intensity in the last three terms on the l.h.s. of Eq. (317), corresponding to frequency derivatives, being given by the "old" values of the specific intensity. In practice, Eq. (317) can be simplified to the ordinary form,

$$-\alpha_{id}J_{i,d-1} - \gamma_{id}J_{i,d+1} + (\beta_{id} + 1 - \widetilde{B}_{id})J_{id} = \epsilon_{id}S_{id}^{\rm th}. \tag{319}$$

where

$$\widetilde{B}_{id} = \mathcal{B}'_{id} + \mathcal{A}_{id}J_{i-1,d}^{\rm old} + \mathcal{C}_{id}J_{i+1,d}^{\rm old}. \tag{320}$$

The numerical solution of this problem is analogous to the solution of the standard problem without Compton scattering; the only difference being that different coefficients enter in the linear equation. Obviously, the explicit solution can be performed frequency by frequency.

It should be kept in mind that regardless whether the implicit or explicit way is used, one still has to iterate to update (i) coefficient $\mathcal{B}'_{id}$ that describes the stimulated emission and which depends on the radiation intensity, and (ii) the Eddington factor. If one uses an explicit method, one has to introduce another nested iteration loop to update coefficient $\widetilde{B}_{id}$ that accounts for the frequency derivatives, and also depends on radiation intensities.

To update the Eddington factor, one has to solve an angle-dependent transfer equation for the specific intensity. To this end, we use the explicit form of the scattering term. As in the standard case, one takes the source function as angle-independent (that is, angle averaged), but unlike the standard case it is taken as known, without an explicit integration of the specific intensity over angle. Therefore, one solves the transfer equation for one frequency-angle point at a time, viz.

$$\mu_j \frac{dI_{ij}}{d\tau_i} = I_{ij} - \epsilon_i S_I^{\text{th}} - \widetilde{B}_i J_i^{\text{old}}, \tag{321}$$

where I_{ij} is the specific intensity at frequency point i and discretized angle point j; μ_j is the cosine of the polar angle. One can employ equation (321) as is, when using the DFE method for the formal solver, or use the second-order (Feautrier) form,

$$\mu_j^2 \frac{d^2 j_{ij}}{d\tau_i^2} = j_{ij} - \epsilon_i S_I^{\text{th}} - \widetilde{B}_i J_i^{\text{old}}, \tag{322}$$

where $j_{ij} \equiv [I_i(\mu_j) + I_i(-\mu_j)]/2$ is the symmetrized (Feautrier) intensity.

Appendix B. Details of the global formal solution

B1. Preconditioned kinetic equilibrium equations

As mentioned in §3.8.2, the crucial part of the global formal solution, i.e., the bulk of calculations performed between the two successive iterations of the linearization scheme, is the simultaneous solution of the radiative transfer and kinetic equilibrium equations, keeping the current atmospheric structure (temperature, density) fixed—the so-called "restricted NLTE problem".

As mentioned above, one can use a simple Lambda iteration scheme, that is to perform an iterative solution that alternates between solving the transfer equation for the current values of level populations, and solving the kinetic equilibrium equations with the current values of radiation intensities. However, there is a much better scheme that is based on the ALI scheme with preconditioning of the kinetic equilibrium, first suggested by Rybicki & Hummer (1991, 1992). We follow here a slightly modified formalism, presented in Hubeny & Mihalas (2014, §14.5).

We use a variant of the scheme, called "preconditioning within the same transition only", in which the discretized kinetic equilibrium equations, with corresponding quadrature weights, denoted in the section as $\overline{w}_i$ to avoid confu-

sion with occupation probabilities, are written as

$$
\begin{aligned}
\sum_l n_l C_{lu} \;+\;& \sum_l \sum_i \overline{w}_i \frac{4\pi}{h\nu_i} \Big(n_l U_{lu} + n_l V_{lu} \Lambda_i [\eta_i^{\mathrm{old}}/\chi_i^{\mathrm{old}}] \\
& -\; n_l V_{lu} \Lambda_i^* [n_u^{\mathrm{old}} U_{ul}/\chi_i^{\mathrm{old}}] - n_l V_{lu} \Lambda_i^* [n_l^{\mathrm{old}} U_{lu}/\chi_i^{\mathrm{old}}] \\
& +\; n_l^{\mathrm{old}} V_{lu} \Lambda_i^* [n_u U_{ul}/\chi_i^{\mathrm{old}}] + n_l^{\mathrm{old}} V_{lu} \Lambda_i^* [n_l U_{lu}/\chi_i^{\mathrm{old}}] \Big) \\
=\sum_l n_u C_{ul} \;+\;& \sum_l \sum_i \overline{w}_i \frac{4\pi}{h\nu_i} \Big(n_u U_{ul} + n_u V_{ul} \Lambda_i [\eta_i^{\mathrm{old}}/\chi_i^{\mathrm{old}}] \\
& -\; n_u V_{ul} \Lambda_i^* [n_l^{\mathrm{old}} U_{lu}/\chi_i^{\mathrm{old}}] - n_u V_{ul} \Lambda_i^* [n_u^{\mathrm{old}} U_{ul}/\chi_i^{\mathrm{old}}] \\
& +\; n_u^{\mathrm{old}} V_{ul} \Lambda_\nu^* [n_l U_{lu}/\chi_i^{\mathrm{old}}] + n_u^{\mathrm{old}} V_{ul} \Lambda_i^* [n_u U_{ul}/\chi_i^{\mathrm{old}}] \Big), \quad (323)
\end{aligned}
$$

where for bound-bound transitions (generalizing the Rybicki & Hummer expressions to include the occupation probabilities w_l and w_u),

$$
\begin{aligned}
U_{ul}(\nu) &\equiv (h\nu/4\pi) A_{ul} \phi_{lu}(\nu) w_l, \quad u > l, & (324) \\
U_{lu}(\nu) &\equiv 0, \quad u > l, & (325) \\
V_{lu}(\nu) &\equiv (h\nu/4\pi) B_{lu} \phi_{lu}(\nu) w_u, & (326)
\end{aligned}
$$

and for bound-free transitions, and for $u > l$,

$$
\begin{aligned}
U_{ul}(\nu) &\equiv n_{\mathrm{e}} \Phi_{ul}(T)(2h\nu^3/c^2)\exp(-h\nu/kT)\sigma_{lu}(\nu) w_l, & (327) \\
U_{lu}(\nu) &\equiv 0, & (328) \\
V_{ul}(\nu) &\equiv n_{\mathrm{e}} \Phi_{ul}(T)\exp(-h\nu/kT)\sigma_{lu}(\nu) w_l, & (329) \\
V_{lu}(\nu) &\equiv \sigma_{lu}(\nu) w_u, & (330)
\end{aligned}
$$

Equations (323) form a linear set for the level populations $n_u, u = 2, \ldots, NL$. The linearity is achieved by considering some level populations in the bi-linear products as the "old" populations. Similarly, the total opacity χ_i that enters in the action of the Λ^* operator, is evaluated using the old populations.

Recognizing that $\Lambda_i^* [\eta_i^{\mathrm{old}}/\chi_i^{\mathrm{old}}] = J_i^{\mathrm{old}}$, and noting that for a diagonal Λ^* operator the terms $-n_l V_{lu} \Lambda_i^* [n_l^{\mathrm{old}} U_{lu}/\chi_i^{\mathrm{old}}]$ and $n_l^{\mathrm{old}} V_{lu} \Lambda_i^* [n_l U_{lu}/\chi_i^{\mathrm{old}}]$ exactly cancel out (and analogously for the term with $n_u n_u^{\mathrm{old}}$), we can rewrite Eq. (323) into a more traditional form,

$$
\sum_{l\neq u} n_l (C_{lu} + R'_{lu}) = n_u \sum_{l\neq u} (C_{ul} + R'_{ul}), \qquad (331)
$$

where, for $l < u$

$$
\begin{aligned}
R'_{lu} &= \sum_i \overline{w}_i \sigma_{lu}(\nu_i) J'_i w_u, & (332) \\
R'_{ul} &= \sum_i \overline{w}_i \sigma_{lu}(\nu_i)\left(J_i + \beta'_i\right) G_{lu}, & (333)
\end{aligned}
$$

67

which are quite parallel to the original equations (65) and (66), replacing J by J' and $\beta = (2h\nu^3/c^2)$ by β', where

$$
\begin{aligned}
J_i' &= J_i - \Lambda_i^* n_u^{\text{old}} U_{ul}/\chi_i^{\text{old}}, &(334)\\
\beta_i' &= (2h\nu_i^3/c^2)[1 - \Lambda_i^* n_l^{\text{old}} \sigma_{lu}(\nu_i) w_u/\chi_i^{\text{old}}]. &(335)
\end{aligned}
$$

One proceeds in exactly the same way as in the ordinary Lambda iteration. The iteration loop consists in solving the transfer equation with the current populations to obtain a better estimate of the mean intensities, and then solving the system (323) or (331) with these mean intensities to obtain the "new" populations n_i. Unlike the ordinary Lambda iteration, the modified radiative rates contain not only the current mean intensities of radiation, but also the approximate operator Λ^* and the "old" populations, known from the previous iteration. The iteration process may be augmented by an application of the Ng acceleration.

Usually, one does not perform many iterations because the aim of the procedure is only to provide an improved and more consistent values of mean intensities and level populations before entering the next step of the global iteration process. But if the procedure is used, for instance, to obtain an exact solution for the radiation field and level populations for a fixed atmospheric structure, then one should perform more iterations of the preconditioning scheme together with Ng acceleration.

The iteration scheme to obtain new populations and mean intensities of radiation, being a classical Lambda iterations or a preconditioning scheme with ALI, is usually supplemented by a simultaneous solution of the charge conservation equation. This is done iteratively; one simply alternates between the solution of the (preconditioned) kinetic equilibrium equations, e.g., Eq. (331), for new populations with a given electron density, and the solution of the charge conservation equation (80) for a new electron density with given populations.

B2. Temperature correction in the convection zone

If the convection is taken into account, the logarithmic gradient ∇, in a discretized form, is given either by

$$
\nabla_d \equiv \nabla_{d-1/2} = \frac{T_d - T_{d-1}}{P_d - P_{d-1}} \frac{P_d + P_{d-1}}{T_d + T_{d-1}}. \tag{336}
$$

or by

$$
\nabla_d = \ln(T_d/T_{d-1})/\ln(P_d/P_{d-1}). \tag{337}
$$

The energy balance equation is linearized as described in detail in Appendix D1; see also Hubeny & Mihalas (2014, § 18.2). Although the linearization scheme may in principle converge without additional correction procedures, in practice it is a very rare situation. The essential point is that a linearization iteration may yield the actual values of temperature and other state parameters such that, for instance, the actual logarithmic gradient in a former convection zone

may spuriously decrease below the adiabatic gradient at certain depth points, so that these points would be declared as convectively stable and the radiative flux would be demanded to be equal to the total flux, which would lead to a serious destabilization of the overall scheme, likely ending in a fatal divergence.

It is therefore almost always necessary to perform certain correction procedures to assure that the convection zone is not disturbed by non-convective regions, and that the temperature and other state parameters are smooth enough functions of depth before one enters the next iteration of the overall linearization scheme. TLUSTY offers several such schemes:

● Definition of the convection zone.
After a completed iteration, the code examines the depth point in which the actual gradient surpasses the adiabatic one. If such a point is solitary, or if it occurs at much smaller column densities than the upper edge of the previous convection zone, the point is declared as convectively stable, and the traditional radiative equilibrium equation is solved for it in the next iteration step. On the other hand, if there is/are depth points in which $\nabla < \nabla_{\rm ad}$ (so that they are seemingly convectively stable), surrounded on both sides by points that are convectively unstable $\nabla \geq \nabla_{\rm ad}$, these points are declared as convectively unstable, and are considered to be part of the convection zone. Within such a newly defined convection zone, one or both of the following correction procedures are performed:

● Standard correction procedure.
The idea of the correction is as follows. In view of Eq. (20), the convective flux is given by

$$F_{\rm conv} = F_0 (\nabla - \nabla_{\rm el})^{3/2},\qquad(338)$$

where

$$F_0 = (gQH_P/32)^{1/2}(\rho c_P T)(\ell/H_P)^2,\qquad(339)$$

After a completed iteration of the global linearization scheme, one takes the current values of the state parameters and the radiation flux, and computes, in the convection zone, the new convective flux corresponding to this radiation flux so that the total flux is perfectly conserved,

$$F^*_{\rm conv} = F_{\rm tot} - F_{\rm rad},\qquad(340)$$

where $F_{\rm tot} = \sigma T^4_{\rm eff}$. If $F_{\rm rad}$ is spuriously larger than $F_{\rm tot}$, then $F_{\rm rad}$ is set to $0.999 F_{\rm tot}$. The new difference of temperature gradients corresponding to this convective flux is then

$$\nabla - \nabla_{\rm el} = (F^*_{\rm conv}/F_0)^{2/3},\qquad(341)$$

which is related to $\nabla - \nabla_{\rm ad}$ through

$$\nabla - \nabla_{\rm ad} = (\nabla - \nabla_{\rm el}) + B\sqrt{\nabla - \nabla_{\rm el}}.\qquad(342)$$

where B is given by Eq. (22). Both B and $\nabla_{\rm ad}$ are computed through the current values of the state parameters. Equation (342) thus yields the new

gradient ∇ and, keeping pressure fixed, the new temperature. With the new temperature, one recalculates the thermodynamic variables, and iterates the process defined by Eqs. (339) - (342) to convergence.

In solving Eq. (342), one proceeds from the top of the convection zone to the bottom, because the gradient ∇ is given by Eq. (336) or (337), so in order to evaluate T_d one needs to know T_{d-1} in the previous depth point.

This procedure works well if the convective flux is dominant, because it should be kept in mind that the radiation flux is also imperfect. Therefore, the temperature is corrected only at depths where the convective flux is larger than some limiting value, $F_{\text{conv}} > \gamma F_{\text{tot}}$, where γ is by default taken as $\gamma = 0.7$, or is set by input data – see Paper III, § 7.8.

- Refined correction procedure

The above procedure is improved by recognizing that the coefficient B is an explicit function of temperature, so B can be expressed as $B \equiv \beta T^3$. More importantly, the radiation flux is not kept fixed, but is written as

$$F_{\text{rad}} \equiv \alpha T^4 \nabla, \tag{343}$$

so that instead of keeping F_{rad} fixed, one first computes α from (343) for the current values of T and ∇, and rewrites the combined equations (340) –(342) as a non-linear equation for the temperature,

$$\nabla(T) = \nabla_{\text{ad}} + \left(\frac{F_{\text{tot}} - \alpha T^4 \nabla(T)}{F_0} \right)^{2/3} + \beta T^3 \left(\frac{F_{\text{tot}} - \alpha T^4 \nabla(T)}{F_0} \right)^{1/3}, \tag{344}$$

which is solved by the Newton-Raphson method, again going from the top of the convection zone to the bottom. This procedure, if chosen to be performed, is done after first completing the standard procedure described above, and only after a certain number of global linearization iterations (driven by input data – see Paper III, § 7.8 and § 12.6).

Other, more sophisticated refinement procedures are in principle possible, but they were not yet implemented in TLUSTY.

B3. Evaluation of the thermodynamic quantities

The internal energy per unit volume is given by

$$E = \frac{3}{2} NkT + 3P_{\text{rad}} + \sum_I N_I \left[E_I + \left(\frac{d \ln U_I}{d \ln T} \right) kT \right], \tag{345}$$

where N_I, U_I, and E_I are the total population, partition function, and the ground state energy (measured from the ground state of the neutral atom) of an ion I, respectively. The latter is thus given by the sum of ionization energies of all the lower ions.

Here, and in the following expressions, it is assumed that the relation between the radiation energy and pressure is given by the equilibrium relation, $E_{\text{rad}} = 3P_{\text{rad}}$, and $P_{\text{rad}} = (a_R/3)T^4$, where a_R is the radiation constant. This

approximation is made only for the purposes of describing convection. The rationale for this approach is that in the situations when convection is important (typically for cool models), the radiation pressure is usually a small part of the total pressure.

The adiabatic gradient is given by

$$\nabla_{\text{ad}} = \left(\frac{\partial \ln T}{\partial \ln P}\right)_S = -\frac{P}{\rho c_P T}\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P, \tag{346}$$

where the specific heat is

$$
\begin{aligned}
c_P &= \left(\frac{\partial E}{\partial T}\right)_P - \frac{P}{\rho^2}\left(\frac{\partial \rho}{\partial T}\right)_P \\
&= \left(\frac{\partial E}{\partial T}\right)_{P_{\text{gas}}} - \left(\frac{\partial E}{\partial P_{\text{gas}}}\right)_T\left(\frac{\partial P}{\partial T}\right)_{P_{\text{gas}}} \\
&\quad - \frac{P}{\rho^2}\left[\left(\frac{\partial \rho}{\partial T}\right)_{P_{\text{gas}}} - \left(\frac{\partial \rho}{\partial P_{\text{gas}}}\right)_T\left(\frac{\partial P}{\partial T}\right)_{P_{\text{gas}}}\right], \tag{347}
\end{aligned}
$$

and

$$\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P = \frac{T}{\rho}\left[\left(\frac{\partial \rho}{\partial T}\right)_{P_{\text{gas}}} - \left(\frac{\partial \rho}{\partial P_{\text{gas}}}\right)_T\left(\frac{\partial P}{\partial T}\right)_{P_{\text{gas}}}\right]. \tag{348}$$

In view of the above approximations, $(\partial P/\partial T)_{P_{\text{gas}}} = 1$, and so all the quantities are expressed in terms of four thermodynamic derivatives, $(\partial E/\partial T)_{P_{\text{gas}}}$, $(\partial E/\partial P_{\text{gas}})_T$, $(\partial \rho/\partial T)_{P_{\text{gas}}}$, $(\partial \rho/\partial P_{\text{gas}})_T$. These derivatives are calculated as differences, e.g., $(\partial E/\partial T)_{P_{\text{gas}}} = [E(T + \Delta T, P_{\text{gas}}) - E(T, P_{\text{gas}})]/\Delta T$, where $\Delta T = 0.001T$.

The thermodynamic quantities may also be formulated through the entropy; which is set by the keyword IFENTR. In this case

$$\nabla_{\text{ad}} = -\left(\frac{\partial S}{\partial T}\right)_{P_{\text{gas}}} \bigg/ \left(\frac{\partial S}{\partial P_{\text{gas}}}\right)_T \frac{P_{\text{gas}}}{T}, \tag{349}$$

and

$$c_P = -\frac{P}{\rho T}\left(\frac{\partial \ln \rho}{\partial \ln T}\right)_P \bigg/ \nabla_{\text{ad}} \tag{350}$$

B4. Recalculation of vertical distance and density for accretion disks

For computing the vertical structure of accretion disks, in which case the gravity acceleration depends on the vertical distance from the central plane, it is important to recalculate the vertical distance and density to be as consistent with the rest of the structural parameters as possible. TLUSTY uses one of the two following procedures:

- Original procedure.

In order to update z, one can use the z-m relation (12), written in a discretized form

$$z_d = z_{d+1} + (m_{d+1} - m_d)(1/\rho_d + 1/\rho_{d+1})/2, \quad z_{ND} = 0. \tag{351}$$

However, using this equation is not convenient in the case where z determined by the current linearization step exhibits an oscillatory or other unphysical behavior. The reason is that Eq. (351) was used in the linearization, so that any such behavior of z was likely shared by a similar behavior of ρ, and thus solving Eq. (351) again does not necessarily help.

A better possibility is to employ a discretized hydrostatic equilibrium equation, used as an equation for z, namely

$$Q(z_d + z_{d+1})/2 = (P_{d+1} - P_d)/(m_{d+1} - m_d), \tag{352}$$

or

$$z_d = \frac{2}{Q} \frac{P_{d+1} - P_d}{m_{d+1} - m_d} - z_{d+1}; \quad z_{ND} = 0, \tag{353}$$

which follows from equation (53). This equation can also be discretized as

$$z_d = \frac{1}{2Q} \left(\frac{P_{d+1} - P_d}{m_{d+1} - m_d} + \frac{P_d - P_{d-1}}{m_d - m_{d-1}} \right). \tag{354}$$

Here, $P = P^{\mathrm{rad}} + P^{\mathrm{gas}}$ is the total pressure; we do not consider an ill-defined turbulent pressure.

An iterative scheme to update the vertical distance and the density proceeds as follows:

(i) Compute the gradient of the radiation pressure as

$$\frac{P_d^{\mathrm{rad}} - P_{d-1}^{\mathrm{rad}}}{m_d - m_{d-1}} = \frac{4\pi}{c} \frac{1}{m_d - m_{d-1}} \sum_{i=1}^{NF} w_i (f_{di} J_{di} - f_{d-1,i} J_{d-1,i}), \tag{355}$$

which is then being held fixed in the subsequent iteration scheme.

(ii) Compute the gas pressure for the current density and electron density as

$$P_d^{\mathrm{gas}} = kT_d N_d = kT_d[\rho_d/(\mu m_H) + n_{\mathrm{e},d}], \tag{356}$$

(iii) Compute a new vertical distance z using Eq. (354). If this procedure yields an unphysical values of z such as $z_d < z_{d+1}$ at certain depth d, one switches to an evaluation of the new $x = z$ using Eq. (353).

(iv) Having determined a new z-scale, recalculate the mass density for $d < ND$ by using Eq. (351), namely

$$\rho_d = \frac{\Delta m_{d+1/2} \rho_{d+1}}{(z_d - z_{d+1})\rho_{d+1} - \Delta m_{d+1/2}}, \tag{357}$$

where $\Delta m_{d+1/2} = (m_{d+1} - m_d)/2$. Before applying Eq. (357), one computes the ratio $\xi_d = n_{\mathrm{e},d}/\rho_d$. After computing new ρ_d for all $d < ND$ from Eq. (357),

one computes new electron density as $n_{e,d} = \xi_d \rho_d$, which is based on a reasonable assumption that the ionization structure is not changed significantly by updating the density.

(v) Steps (ii) - (iv) are repeated until a relative change in z is sufficiently small.

• Modified procedure.

A better overall procedure is to solve simultaneously six governing equations for the six unknowns that form a vector ψ_d, viz.

$$\psi_d \equiv \{P_d, P_d^{gas}, \rho_d, N_d, n_{e,d}, z_d\}, \tag{358}$$

where, at depth point d, P_d is the total pressure, N_d is the total particle number density. and the other symbols have their usual meaning. The six governing equations are

$$(P_d - P_{d-1})/\Delta m_{d-1/2} - Q(z_d + z_{d-1}) = 0, \tag{359}$$
$$P_d - P_d^{gas} - P_d^{rad} = 0, \tag{360}$$
$$\rho_d - (\mu/m_H)(N_d - n_{e,d}) = 0, \tag{361}$$
$$P_d^{gas} - N_d k T_d = 0, \tag{362}$$
$$n_{e,d} - \zeta_d N_d = 0, \tag{363}$$
$$z_d - z_{d+1} - \Delta m_{d+1/2}(1/\rho_d + 1/\rho_{d+1}) = 0. \tag{364}$$

The first equation apply for $d > 1$. For $d = 1$ it is replaced by (for details refer to Appendix D.2),

$$\rho_1 H_g f(x_1) - m_1 = 0, \tag{365}$$

and the last equation for $d = ND$ is replaced by

$$z_{ND} = 0. \tag{366}$$

The non-linear set of equations (359) - (366) is solved by linearization for the six components of vector ψ. The resulting set of linearized equations can be written as

$$-A_d \delta\psi_{d-1} + B_d \delta\psi_d - C_d \delta\psi_{d+1} = L_d, \tag{367}$$

where A_d, B_d, and C_d are 6×6 matrices. The system (367) is solved by a standard Gauss-Jordan forward-backward elimination scheme described by Eqs. (123) - (125). The temperature T_d and the radiation pressure P_d^{rad} are held fixed. The ratio $\zeta_d = n_{e,d}/N_d$ is recomputed after each internal iteration step and is held constant during the next one.

From the physical point of view, the above procedure is equivalent to the original one, as it solves the hydrostatic equilibrium equation together with the $z - m$ relation (the rest of the six governing equations are essentially the definitions of the individual quantities), but the iteration scheme to obtain the solution is more efficient in the presert procedure.

Appendix C. Linearization of the structural equations

Notation

The order of the individual quantities in the state vector ψ, and the order of equations within the global operator $\mathbf{P}$ are arbitrary. Here we chose, in keeping with the original approach introduced in Auer & Mihalas (1969), the state vector in the form (118), and the corresponding order of equations: NF transfer equations for explicit (linearized) frequency points, hydrostatic equilibrium equation, radiative equilibrium equation, charge conservation equation, and NL kinetic equilibrium equations supplemented by the corresponding particle conservation (abundance definition) equations. To simplify the notation, the index corresponding to hydrostatic equilibrium (or total particle density N) is denoted NH; the index corresponding to radiative equilibrium (or temperature T) as NR, and that corresponding to charge conservation (and the electron density n_{e}) as NP. In the present convention

$$NH = NF + 1, \quad NR = NF + 2, \quad NP = NF + 3. \tag{368}$$

in the case of accretion disks, there is another state parameter and corresponding equation, namely the geometrical distance from the midplane, z. The corresponding index is denoted NZ, and its usual value is $NZ = NF + 4$.

However, TLUSTY can accept any reasonable values for these parameters, not just those specified by Eq. (368).

C1. Stellar atmospheres

Linearized transfer equation

The discretized transfer equation was already considered in Appendix A, and is described by Eqs. (215) - (220). Let $i, i = 1, \ldots, NF$, be a row corresponding to the transfer equation, and let $P_i(\psi) = \mathbf{0}$ be a formal expression of the transfer equation. Then the individual matrix element ij represents the partial derivative of the i-th transfer equation with respect to the j-th mean intensity,

- For the upper boundary condition, $d = 1$, and $j = 1, \ldots, NF$

$$(B_1)_{ij} \quad \equiv \quad \frac{\partial P_{1,i}}{\partial J_{1,j}} = \left[\frac{f_{1,i}}{\Delta\tau_{3/2,i}} + g_i + \frac{\tau_{3/2,i}}{2}\epsilon_{1,i} \right] \delta_{ij}, \tag{369}$$

$$(C_1)_{ij} \quad \equiv \quad -\frac{\partial P_{1,i}}{\partial J_{2,j}} = \frac{f_{2,i}}{\Delta\tau_{3/2,i}} \delta_{ij}. \tag{370}$$

The other columns corresponding to the components $\psi_{d,k}$, for $k > NF$, i.e. corresponding to the temperatures and the number densities (total, electron,

and level populations)

$$(B_1)_{ik} \equiv \frac{\partial P_{1,i}}{\partial \psi_{1,k}} = \left[-\frac{f_{1,i}J_{1,i} - f_{2,i}J_{2,i}}{\Delta\tau_{3/2,i}^2} + \frac{1}{2}\left(\epsilon_{1,i}J_{1,i} - \frac{\eta_{1,i}}{\chi_{1,i}}\right)\right]\frac{\partial\Delta\tau_{3/2,i}}{\partial\psi_{1,k}}$$
$$+ \frac{\Delta\tau_{3/2,i}}{2}\left[\frac{\partial\epsilon_{1,i}}{\partial\psi_{1,k}}J_{1,i} - \frac{\eta_{1,i}}{\chi_{1,i}}\left(\frac{1}{\eta_{1,i}}\frac{\partial\eta_{1,i}}{\partial\psi_{1,k}} - \frac{1}{\chi_{1,i}}\frac{\partial\chi_{1,i}}{\partial\psi_{1,k}}\right)\right], \quad (371)$$

$$(C_1)_{ik} \equiv -\frac{\partial P_{1,i}}{\partial\psi_{2,k}} = \left(\frac{f_{1,i}J_{1,i} - f_{2,i}J_{2,i}}{\Delta\tau_{3/2,i}^2}\right)\frac{\partial\Delta\tau_{3/2,i}}{\partial\psi_{2,k}}, \quad (372)$$

where, generally,

$$\frac{\partial\Delta\tau_{d-1/2,i}}{\partial\psi_{d,k}} = \frac{\Delta\tau_{d-1/2,i}}{\omega_d + \omega_{d-1}}\frac{\partial\omega_{d-1,i}}{\partial\psi_{d-1,k}}, \quad (373)$$

and $\omega_{di} = \chi_{di}/\rho_d$. The components of the right-hand side vector $\mathbf{L}_1$ are given by

$$L_{1i} \equiv -P_{1,i} = -\frac{f_{1,i}J_{1,i} - f_{2,i}J_{2,i}}{\Delta\tau_{3/2,i}} - g_iJ_{1,i} + H_i^{\text{ext}} - \frac{\Delta\tau_{3/2,i}}{2}\left(\epsilon_{1,i}J_{1,i} - \frac{\eta_{1,i}}{\chi_{1,i}}\right). \quad (374)$$

• For the inner points, $d = 2, \dots, ND - 1$, one has for $j = 1, \dots, NF$,

$$(A_d)_{ij} = \frac{f_{d-1,i}}{\Delta\tau_{d-1/2,i}\Delta\tau_{d,i}}\delta_{ij}, \quad (375)$$

$$(B_d)_{ij} = \left[\frac{f_{d,i}}{\Delta\tau_{d,i}}\left(\frac{1}{\Delta\tau_{d-1/2,i}} + \frac{1}{\Delta\tau_{d+1/2,i}}\right) + \epsilon_{d,i}\right]\delta_{ij}, \quad (376)$$

$$(C_d)_{ij} = \frac{f_{d+1,i}}{\Delta\tau_{d+1/2,i}\Delta\tau_{d,i}}\delta_{ij}, \quad (377)$$

and for $k > NF$,

$$(A_d)_{ik} = a_{di}\frac{\partial\omega_{d-i,i}}{\partial\psi_{d-1,k}}, \quad (378)$$

$$(C_d)_{ik} = c_{di}\frac{\partial\omega_{d+1,i}}{\partial\psi_{d+1,k}}, \quad (379)$$

$$(B_d)_{ik} = -(a_{di} + c_{di})\frac{\partial\omega_{d,i}}{\partial\psi_{d,k}} + \frac{\partial\epsilon_{1,i}}{\partial\psi_{1,k}}J_{di}$$
$$- \frac{\eta_{d,i}}{\chi_{d,i}}\left(\frac{1}{\eta_{d,i}}\frac{\partial\eta_{d,i}}{\partial\psi_{d,k}} - \frac{1}{\chi_{d,i}}\frac{\partial\chi_{d,i}}{\partial\psi_{d,k}}\right), \quad (380)$$

where

$$\alpha_{di} = \frac{f_{di}J_{di} - f_{d-1,i}J_{d-1,i}}{\Delta\tau_{d-1/2,i}\Delta\tau_{di}}, \quad (381)$$

$$\gamma_{di} = \frac{f_{di}J_{di} - f_{d+1,i}J_{d+1,i}}{\Delta\tau_{d+1/2,i}\Delta\tau_{di}}, \quad (382)$$

$$\beta_{di} = \alpha_{di} + \gamma_{di}, \tag{383}$$

$$a_{di} = \left[\alpha_{di} + (1/2)\beta_{di}(\Delta\tau_{d-1/2,i}/\Delta\tau_{di})\right]/\left(\omega_{d-1,i} + \omega_{di}\right), \tag{384}$$

$$c_{di} = \left[\gamma_{di} + (1/2)\beta_{di}(\Delta\tau_{d+1/2,i}/\Delta\tau_{di})\right]/\left(\omega_{d+1,i} + \omega_{di}\right), \tag{385}$$

and the right–hand–side vector

$$L_{di} = -\beta_{di} - \epsilon_{di}J_{di} + \eta_{di}/\chi_{di}. \tag{386}$$

• For the lower boundary condition, $d = ND$, we have, for $j \leq NF$, $k > NF$,

$$(B_d)_{ij} = \left[\frac{f_{di}}{\Delta\tau_{d-1/2,i}} + \frac{1}{2} + \frac{\tau_{d-1/2,i}}{2}\epsilon_{di}\right]\delta_{ij}, \tag{387}$$

$$(A_d)_{ij} = \frac{f_{d-1,i}}{\Delta\tau_{d-1/2,i}}\delta_{ij}, \tag{388}$$

$$\begin{aligned}
(B_d)_{ik} &= \left[-\frac{f_{di}J_{di} - f_{d-1,i}J_{d-1,i}}{\Delta\tau_{d-1/2,i}^2} + b_i + \frac{1}{2}\left(\epsilon_{di}J_{di} - \frac{\eta_{di}}{\chi_{di}}\right)\right]\frac{\partial\Delta\tau_{d-1/2,i}}{\partial\psi_{d,k}} \\
&+ \frac{\Delta\tau_{d-1/2,i}}{2}\left[\frac{\partial\epsilon_{di}}{\partial\psi_{d,k}}J_{di} - \frac{\eta_{di}}{\chi_{di}}\left(\frac{1}{\eta_{di}}\frac{\partial\eta_{di}}{\partial\psi_{d,k}} - \frac{1}{\chi_{di}}\frac{\partial\chi_{di}}{\partial\psi_{d,k}}\right)\right] \\
&- \left(\frac{1}{2} + \frac{1}{3\Delta\tau_{d-1/2,i}}\right)\left(\frac{dB_i}{dT}\right)_d\delta_{k,NR},
\end{aligned} \tag{389}$$

$$\begin{aligned}
(A_d)_{ik} &= \left(\frac{f_{di}J_{di} - f_{d-1,i}J_{d-1,i}}{\Delta\tau_{d-1/2,i}^2} - b_i\right)\frac{\partial\Delta\tau_{d-1/2,i}}{\partial\psi_{d-1,k}} \\
&- \frac{1}{3\Delta\tau_{d-1/2,i}}\left(\frac{dB_i}{dT}\right)_{d-1}\delta_{k,NR},
\end{aligned} \tag{390}$$

where

$$b_i \equiv \frac{1}{3}\frac{B_{di} - B_{d-1,i}}{\Delta\tau_{d-1/2,i}^2}. \tag{391}$$

The last terms in Eqs.(389) and (390), which only apply for $\psi_k = T$, i.e., $k = NR$, arise from the derivatives of the Planck function with respect to temperature. Finally

$$\begin{aligned}
L_{d,i} &= -\frac{f_{di}J_{di} - f_{d-1,i}J_{d-1,i}}{\Delta\tau_{d-1/2,i}} - \frac{1}{2}(J_{di} - B_{di}) + \frac{1}{3}\frac{B_{di} - B_{d-1,i}}{\Delta\tau_{d-1/2,i}} \\
&- \frac{\Delta\tau_{d-1/2,i}}{2}\left(\epsilon_{di}J_{di} - \frac{\eta_{di}}{\chi_{di}}\right).
\end{aligned} \tag{392}$$

Linearized hydrostatic equilibrium equation

The discretized form of Eq. (15) reads

$$N_dkT_d - N_{d-1}kT_{d-1} + \frac{4\pi}{c}\sum_{i=1}^{NF}w_i(f_{di}J_{di} - f_{d-1,i}J_{d-1,i}) = g(m_d - m_{d-1}). \tag{393}$$

The upper boundary condition is derived from Eq. (15) assuming that the radiation force remains constant from the boundary surface upward:

$$N_1 k T_1 = m_1 \big[g - (4\pi/c) \sum_{i=1}^{NF} w_i (\chi_{1i}/\rho_1) g_i J_{1i} \big]. \tag{394}$$

For accretion disks, Eqs. (393) and (394) remain unchanged, the only difference is in the expression for the gravity acceleration g as

$$g \equiv g(z) = Q(z_d + z_{d-1})/2. \tag{395}$$

The upper boundary condition is given by Eqs. (189) and (190).

The components of matrices $\mathbf{A}$, $\mathbf{B}$, and vector $\mathbf{L}$ corresponding to the hydrostatic equilibrium equation, the row $NH = NF + 1$, follow from linearizing Eqs. (393) and (394), are given by

$$(B_1)_{NH,i} = (4\pi/c)\, w_i \omega_{1,i} g_i, \quad i \leq NF, \tag{396}$$

$$(B_1)_{NH,NH} = k T_1, \tag{397}$$

$$(B_1)_{NH,NR} = k N_1 + \frac{4\pi}{c} \sum_{j=1}^{NF} w_j g_j J_{1,j} \frac{\partial \omega_{1,j}}{\partial T_1}, \tag{398}$$

$$(B_1)_{NH,n} = \frac{4\pi}{c} \sum_{j=1}^{NF} w_j g_j J_{1,j} \frac{\partial \omega_{1,j}}{\partial \psi_{1,n}}, \; n > NR, \tag{399}$$

$$(L_1)_{NH} = g m_1 - N_1 k T_1 - \frac{4\pi}{c} \sum_{j=1}^{NF} w_j \omega_{1j} g_i J_{1i}, \tag{400}$$

and, for $d > 1$,

$$(A_d)_{NH,i} = (4\pi/c) w_i f_{d-1,i}, \quad i \leq NF, \tag{401}$$

$$(B_d)_{NH,i} = (4\pi/c) w_i f_{di}, \quad i \leq NF, \tag{402}$$

$$(A_d)_{NH,NH} = k T_{d-1}, \tag{403}$$

$$(B_d)_{NH,NH} = k T_d, \tag{404}$$

$$(A_d)_{NH,NR} = k N_{d-1}, \tag{405}$$

$$(B_d)_{NH,NR} = k N_d, \tag{406}$$

$$(L_d)_{NH} = g(m_d - m_{d-1}) - N_d k T_d + N_{d-1} k T_{d-1}$$
$$- \frac{4\pi}{c} \sum_{j=1}^{NF} w_j (f_{di} J_{di} - f_{d-1,i} J_{d-1,i}). \tag{407}$$

Linearized radiative equilibrium equation

By discretizing the radiative equilibrium equation (16) one obtains

$$\alpha_d \sum_{i=1}^{NF} w_i (\kappa_{di} J_{di} - \eta_{di}) + \beta_d \left[\sum_{i=1}^{NF} w_i \frac{f_{di} J_{di} - f_{d-1,i} J_{d-1,i}}{\Delta \tau_{d-1/2,i}} - \frac{\sigma_R}{4\pi} T_{\text{eff}}^4 \right] = 0. \tag{408}$$

For accretion disks, Eq. (408) is modified as expressed in Eq. (59),

$$\alpha_d \left[\sum_{i=1}^{NF} w_i (\kappa_{di} J_{di} - \eta_{di}) + E_{\text{diss,d}} \right]$$

$$+ \beta_d \left[\sum_{i=1}^{NF} w_i \frac{f_{di} J_{di} - f_{d-1,i} J_{d-1,i}}{\Delta \tau_{d-1/2,i}} - \frac{\sigma_R}{4\pi} T_{\text{eff}}^4 (1 - \theta_d) \right] = 0, \tag{409}$$

where E_{diss} and θ are given by Eqs. (60) and (58), respectively.

Linearization of Eq. (408), for $d > 1$ and $k \geq NR$, yields

$$(A_d)_{NR,i} = \beta_d \, w_i \frac{f_{d-1,i}}{\Delta \tau_{d-1/2,j}}, \quad i \leq NF, \tag{410}$$

$$(A_d)_{NR,k} = \beta_d \sum_{j=1}^{NF} w_j \frac{f_{dj} J_{dj} - f_{d-1,j} J_{d-1,j}}{\Delta \tau_{d-1/2,j}^2} \frac{\partial \Delta \tau_{d-1/2,j}}{\partial \psi_{d-1,k}}, \tag{411}$$

$$(B_d)_{NR,i} = \alpha_d w_i \kappa_{di} + \beta_d w_i \frac{f_{di}}{\Delta \tau_{d-1/2,j}}, \quad i \leq NF, \tag{412}$$

$$(B_d)_{NR,k} = \alpha_d \sum_{j=1}^{NF} w_j \left(\frac{\partial \kappa_{dj}}{\partial \psi_{dk}} J_{dj} - \frac{\partial \eta_{dj}}{\partial \psi_{dk}} \right)$$

$$- \beta_d \sum_{j=1}^{NF} w_j \frac{f_{dj} J_{dj} - f_{d-1,j} J_{d-1,j}}{\Delta \tau_{d-1/2,j}^2} \frac{\partial \Delta \tau_{d-1/2,j}}{\partial \psi_{d,k}}, \tag{413}$$

and

$$(L_d)_{NR} = -\alpha_d \sum_{j=1}^{NF} w_j (\kappa_{dj} J_{dj} - \eta_{dj})$$

$$+ \beta_d \left[\frac{\sigma_R}{4\pi} T_{\text{eff}}^4 - \sum_{j=1}^{NF} w_j \frac{f_{dj} J_{dj} - f_{d-1,j} J_{d-1,j}}{\Delta \tau_{d-1/2,j}} \right]. \tag{414}$$

The upper boundary condition for $d = 1$ is

$$(B_d)_{NR,i} = \alpha_d w_i \kappa_{di} + \beta_d w_i g_i, \quad i \leq NF, \tag{415}$$

$$(L_d)_{NR} = -\alpha_d \sum_{j=1}^{NF} w_j (\kappa_{dj} J_{dj} - \eta_{dj})$$

$$+ \beta_d \left[\frac{\sigma_R}{4\pi} T_{\text{eff}}^4 - \sum_{j=1}^{NF} w_j w_j (g_j J_{1j} - H_j^{\text{ext}}) \right]. \tag{416}$$

Linearized charge conservation equations

The equation is local and simple, so the linearization is straightforward

$$(B_d)_{NP,NP} = -1, \tag{417}$$

$$(B_d)_{NP,i} = Z_i, \quad i > NP, \tag{418}$$

where Z_i is the charge of the ion to which level i belongs, and

$$(L_d)_{NP} = n_e - \sum_{i=1}^{NL} n_i Z_i. \tag{419}$$

All other elements of the NP-th row of matrix $\mathbf{B}$, and all elements of the NP-th row of matrices $\mathbf{A}$ and $\mathbf{C}$ are zero.

Linearized kinetic equilibrium equations

The radiative rates are written as quadrature sums,

$$R_{lu} = \frac{4\pi}{h} \sum_{i=1}^{NF} \frac{1}{\nu_i} w_i \sigma_{lu}(\nu_i) J_{di}, \tag{420}$$

$$R_{lu} = \frac{4\pi}{h} \sum_{i=1}^{NF} \frac{1}{\nu_i} w_i \sigma_{lu}(\nu_i) \left(\frac{2h\nu_i^3}{c^2} + J_{di} \right). \tag{421}$$

where the summations formally extend over all frequency points. It should be kept in mind that the appropriate cross-section differ from zero only in limited ranges of frequencies.

The kinetic equilibrium equations (61) are local, therefore $A_{ij} = C_{ij} = 0$ for $i > NP$ and all j. Because the form of matrix elements is the same for all depth points, we drop the depth index d. The matrix elements are as follows

$$B_{m,i} = \sum_{j=1}^{NL} \frac{\partial \mathcal{A}_{mj}}{\partial J_i} n_j, \quad i \le NF, \tag{422}$$

$$B_{m,NR} = \sum_{j=1}^{NL} \frac{\partial \mathcal{A}_{mj}}{\partial T} n_j, \tag{423}$$

$$B_{m,NP} = \sum_{j=1}^{NL} \frac{\partial \mathcal{A}_{mj}}{\partial n_e} n_j, \tag{424}$$

$$B_{mj} = \mathcal{A}_{mj}, \quad j > NP, \tag{425}$$

$$L_m = b_m - \sum_{j=1}^{NL} \mathcal{A}_{mj} n_j. \tag{426}$$

For each atomic species I, the rate equation for a characteristic level, say k, is replaced by the particle conservation equation, (74). The corresponding matrix elements are

$$B_{ki} = 1, \tag{427}$$

$$B_{k,NH} = -\alpha_I, \tag{428}$$

$$B_{k,NP} = \alpha_I, \tag{429}$$

where i labels all levels considered for species I, and $\alpha_I = A_I / \sum_J A_J$ is the fractional abundance of species I.

Linearized equation for convection

When convection is taken into account, it is advantageous to consider the logarithmic gradient of temperature ∇ as one of the state parameters, and include it in the state vector ψ,

$$\psi_d = \{J_{d1}, \ldots, J_{d,NF}, N, T, n_{e,d}, n_{d1}, \ldots, n_{d,NL}, \nabla_d\}, \qquad (430)$$

where we adopt the convention that the gradient ∇_d is the one corresponding to depth $d - 1/2$, i.e.,

$$\nabla_{d-1/2} = (\ln T_d - \ln T_{d-1})/(\ln P_d - \ln P_{d-1}). \qquad (431)$$

The gradient may also be evaluated as

$$\nabla_{d-1/2} = \frac{T_d - T_{d-1}}{T_d + T_{d-1}} \cdot \frac{P_d + P_{d-1}}{P_d - P_{d-1}}. \qquad (432)$$

In the following, we use equation (432) to represent the logarithmic temperature gradient. The corresponding adiabatic gradient also has to be evaluated at the mid-point $d - \frac{1}{2}$, $\nabla_{\mathrm{ad}} = \nabla_{\mathrm{ad}}(T_{d-1/2}, P_{d-1/2})$, with $T_{d-1/2} = (T_d + T_{d-1})/2$, and a similar equation for $P_{d-1/2}$. The mid-point values may also be evaluated as geometric means, i.e. $T_{d-1/2} = (T_d T_{d-1})^{1/2}$, but in the following we use the arithmetic mean. The convective flux is a quantity that also corresponds to the grid mid-points, hence it should be written as $F_{\mathrm{conv}} = F_{\mathrm{conv},d-1/2}$.

At the depth points where the Schwarzschild criterion is satisfied, the radiative equilibrium equation has to be modified to radiative+convective equilibrium equation which reads

$$\alpha_d \left[\sum_i w_i(\kappa_i J_i - \eta_i) + \frac{\rho_d}{4\pi} \frac{F_{d+1/2}^{\mathrm{conv}}(\psi_{\mathbf{d}}, \psi_{d+1}) - F_{d-1/2}^{\mathrm{conv}}(\psi_{\mathbf{d}}, \psi_{d-1})}{\Delta m_d} \right]$$

$$+ \beta_d \left[\sum_{i=1}^{NF} w_i \frac{f_{di} J_{di} - f_{d-1,i} J_{d-1,i}}{\Delta \tau_{d-1/2,i}} - \frac{\sigma_R}{4\pi} T_{\mathrm{eff}}^4 + \frac{F_{d-1/2}^{\mathrm{conv}}(\psi_d, \psi_{d-1})}{4\pi} \right] = 0, \quad (433)$$

where $\Delta m_d = (m_{d+1} - m_{d-1/2})/2$. Here we show explicitly a dependence of the convective flux of the state parameters, because for instance $F_{d-1/2}^{\mathrm{conv}}$ is evaluated at the midpoint, that is, for temperature $T = (T_d + T_{d-1})/2$, and analogously for other quantities. For accretion disks, Eq. (433) is modified analogously to Eq. (409).

There are four modifications of matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and vector $\mathbf{L}$ when convection is taken into account:
– a modification of the row $NR = NF + 2$, corresponding to radiative equilibrium, now being modified to radiative + convective equilibrium;

– an addition of a column in all matrices corresponding to ∇; using the convention of equation (430), it is the column $NN = NF + NL + 4$;

– an addition of a row NN, corresponding to ∇;

– a modification of vector $\mathbf{L}$, namely changing the NR element, and adding the NN element.

$\bullet$ Because the convective flux depends only on T, P, and ∇, and writing $P = NkT$, the only new elements of the row NR of matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$ are those corresponding to N, T, and ∇. In the radiative zone, $\nabla < \nabla_{\mathrm{ad}}$, all new elements are zero. In the convection zone, $\nabla \geq \nabla_{\mathrm{ad}}$, there are the following additions to the matrix elements, denoted by superscript "conv", that follow from linearizing equation (433), where we introduce $H^{\mathrm{conv}} \equiv F^{\mathrm{conv}}/4\pi$,

$$
\begin{aligned}
A_{NR,NH}^{\mathrm{conv}} &= \alpha_d \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} \frac{\rho_d}{2\Delta m_d} kT_{d-1} \\
&+ \frac{\beta_d}{2} \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} kT_{d-1}, \quad (434)
\end{aligned}
$$

$$
\begin{aligned}
A_{NR,NR}^{\mathrm{conv}} &= \alpha_d \left[\left(\frac{\partial H^{\mathrm{conv}}}{\partial T} \right)_{d-1/2} + \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} kN_{d-1} \right] \frac{\rho_d}{2\Delta m_d} \\
&+ \beta_d \left[\frac{1}{2} \left(\frac{\partial H^{\mathrm{conv}}}{\partial T} \right)_{d-1/2} + \frac{1}{2} \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} kN_{d-1} \right], \quad (435)
\end{aligned}
$$

$$
A_{NR,NN}^{\mathrm{conv}} = \alpha_d \frac{H_{d-1/2}^{\mathrm{conv}}}{(\nabla_d - \nabla_{\mathrm{el},d-1/2})} \frac{3\rho_d}{4\Delta m_d}, \quad (436)
$$

$$
\begin{aligned}
B_{NR,NH}^{\mathrm{conv}} &= \alpha_d \left[\left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d+1/2} - \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} \right] \frac{\rho_d}{2\Delta m_d} kT_d \\
&+ \frac{\rho_d}{(N_d - n_{\mathrm{e},d})} \frac{H_{d+1/2}^{\mathrm{conv}} - H_{d-1/2}^{\mathrm{conv}}}{\Delta m_d} \\
&+ \frac{\beta_d}{2} \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} kT_d, \quad (437)
\end{aligned}
$$

$$
\begin{aligned}
B_{NR,NR}^{\mathrm{conv}} &= \alpha_d \left[\left(\frac{\partial H^{\mathrm{conv}}}{\partial T} \right)_{d+1/2} + \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d+1/2} kN_d \right. \\
&- \left. \left(\frac{\partial H^{\mathrm{conv}}}{\partial T} \right)_{d-1/2} - \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} kN_d \right] \frac{\rho_d}{2\Delta m_d} \\
&+ \beta_d \left[\frac{1}{2} \left(\frac{\partial H^{\mathrm{conv}}}{\partial T} \right)_{d-1/2} + \frac{1}{2} \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d-1/2} kN_d \right], \quad (438)
\end{aligned}
$$

$$
B_{NR,NP}^{\mathrm{conv}} = -\alpha_d \frac{\rho_d}{(N_d - n_{\mathrm{e},d})} \frac{H_{d+1/2}^{\mathrm{conv}} - H_{d-1/2}^{\mathrm{conv}}}{\Delta m_d}, \quad (439)
$$

$$
B_{NR,NN}^{\mathrm{conv}} = \alpha_d \left[\frac{H_{d+1/2}^{\mathrm{conv}}}{\nabla_{d+1} - \nabla_{\mathrm{el},d+1/2}} - \frac{H_{d-1/2}^{\mathrm{conv}}}{\nabla_d - \nabla_{\mathrm{el},d-1/2}} \right] \frac{3\rho_d}{4\Delta m_d}
$$

$$+ \quad \beta_d \frac{3}{2} \frac{H^{\mathrm{conv}}_{d-1/2}}{\nabla_d - \nabla_{\mathrm{el},d-1/2}}, \tag{440}$$

$$C^{\mathrm{conv}}_{NR,NH} = -\alpha_d \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d+1/2} \frac{\rho_d}{2\Delta m_d} k T_{d+1}, \tag{441}$$

$$C^{\mathrm{conv}}_{NR,NR} = -\alpha_d \left[\left(\frac{\partial H^{\mathrm{conv}}}{\partial T} \right)_{d+1/2} + \left(\frac{\partial H^{\mathrm{conv}}}{\partial P} \right)_{d+1/2} k N_{d-1} \right] \frac{\rho_d}{2\Delta m_d}, \tag{442}$$

$$C^{\mathrm{conv}}_{NR,NN} = -\alpha_d \frac{H^{\mathrm{conv}}_{d+1/2}}{(\nabla_d - \nabla_{\mathrm{el},d+1/2})} \frac{3\rho_d}{4\Delta m_d}, \tag{443}$$

$$L^{\mathrm{conv}}_{NR} = -\alpha_d \frac{\rho_d}{\Delta m_d} (H^{\mathrm{conv}}_{d+1/2} - H^{\mathrm{conv}}_{d-1/2}) - \beta_d H^{\mathrm{conv}}_{d-1/2}, \tag{444}$$

where we used $\partial T_{d-1/2}/\partial T_d = 1/2$. The partial derivatives of the convective flux with respect to temperature and pressure are obtained numerically,

$$\frac{\partial H^{\mathrm{conv}}}{\partial T} = \frac{H^{\mathrm{conv}}(T + \delta T, P, \nabla) - H^{\mathrm{conv}}(T, P, \nabla)}{\delta T}, \tag{445}$$

and analogously for the derivative with respect to pressure. Here, δT is an arbitrary small quantity; it is typically chosen $\delta T = 0.01\,T$. The derivative with respect to ∇ is computed analytically.

• The additional row corresponding to ∇, that is a linearized equation (432), is simple

$$A^{\mathrm{conv}}_{NN,NH} = -\frac{2P_d \nabla_d}{P_d^2 - P_{d-1}^2} k T_{d-1}, \tag{446}$$

$$A^{\mathrm{conv}}_{NN,NR} = \frac{2T_d \nabla_d}{T_d^2 - T_{d-1}^2} - \frac{2P_d \nabla_d}{P_d^2 - P_{d-1}^2} k N_{d-1}, \tag{447}$$

$$B^{\mathrm{conv}}_{NN,NH} = -\frac{2P_{d-1} \nabla_d}{P_d^2 - P_{d-1}^2} k T_d, \tag{448}$$

$$B^{\mathrm{conv}}_{NN,NR} = \frac{2T_{d-1} \nabla_d}{T_d^2 - T_{d-1}^2} - \frac{2P_{d-1} \nabla_d}{P_d^2 - P_{d-1}^2} k N_d, \tag{449}$$

$$B^{\mathrm{conv}}_{NN,NN} = -1, \tag{450}$$

and

$$L_{NN} = \nabla_d - \frac{T_d - T_{d-1}}{T_d + T_{d-1}} \cdot \frac{P_d + P_{d-1}}{P_d - P_{d-1}}. \tag{451}$$

C2. Accretion disks

Radiative transfer equation

It is the same as for stellar atmospheres; the only difference is in the lower boundary condition, $d = ND$. Its discretized form follows from integrating Eq. (220) over angles. The corresponding matrix elements are given by the same expressions as in Eqs. (387) - (390); the only difference is that in Eqs. (389)

and (390) the specific terms for $k = NR$ are not present; formally it is expressed as the term $\delta_{k,NR} = 0$ for all values of k. The elements of the right-hand side vector are given by

$$L_{d,i} = -\frac{f_{di}J_{di} - f_{d-1,i}J_{d-1,i}}{\Delta\tau_{d-1/2,i}} - \frac{\Delta\tau_{d-1/2,i}}{2}\left(\epsilon_{di}J_{di} - \frac{\eta_{di}}{\chi_{di}}\right). \tag{452}$$

Vertical hydrostatic equilibrium equation

All matrix elements $A_{NH,i}$ and $B_{NH,i}$ and vector L_{NH} remain unchanged, the only difference is the addition of elements corresponding to vertical distance z,

$$(A_d)_{NH,NZ} = Q(m_d - m_{d-1})/2, \tag{453}$$
$$(B_d)_{NH,NZ} = -Q(m_d - m_{d-1})/2 \tag{454}$$

The upper boundary condition can either be considered to be the same as in the case of stellar atmospheres, or is taken in a different form, based on the formalism put forward in §4.2, specifically Eqs. (189) and (190). However, the scale heights H_g and H_r are not approximated, but instead are treated using actual values of the state parameters, and are thus linearized. Specifically,

$$H_g = \left(\frac{2N_1 k T_1}{\rho_1 Q}\right)^{1/2}, \tag{455}$$

$$H_r = \frac{4\pi}{cQ\rho_1}\sum_{i+1}^{NF} w_i\chi_i\left(g_i J_i - H_i^{\text{ext}}\right) \tag{456}$$

The right-hand side is given by

$$(L_1)_{NH} = m_1 - H_g\rho_1 f(x_1), \tag{457}$$

where

$$x_1 = \frac{z_1 - H_r}{H_g}, \quad \text{and} \quad f(x) = \frac{\sqrt{\pi}}{2}\exp(x^2)\text{erfc}(x). \tag{458}$$

and the matrix elements are

$$(B_1)_{NH,i} = -\frac{4\pi}{cQ}f_1' w_i g_i \chi_{1i}, \quad i = 1, \ldots, NF, \tag{459}$$

$$(B_1)_{NH,NH} = \frac{1}{N_1}(\rho_1 H_g f_1 + H_r\rho_1 f_1'), \tag{460}$$

$$(B_1)_{NH,NR} = \frac{1}{2T_1}[\rho_1 H_g f_1 + \rho_1 f_1'(H_r - z_1)]$$
$$- \frac{4\pi}{cQ}f_1'\sum_{i=1}^{NF} w_i\frac{\partial\chi_{1i}}{\partial T_1}\left(g_i J_i - H_i^{\text{ext}}\right), \tag{461}$$

$$(B_1)_{NH,k} = -\frac{4\pi}{cQ}f_1'\sum_{i=1}^{NF} w_i\frac{\partial\chi_{1i}}{\partial\psi_{1k}}\left(g_i J_i - H_i^{\text{ext}}\right), \tag{462}$$

$$(B_1)_{NH,NZ} = \rho_1 f_1', \tag{463}$$

where $k > NR$ and $k \neq NZ$, and

$$f_1 = f(x_1), \quad f'_1 = \left.\frac{df}{dx}\right|_1, \tag{464}$$

and f' is evaluated as $f'(x) = [f(x + \Delta x) - f(x)]/\Delta x$ with $\Delta x = 0.01x$.

Energy balance equation

As follows from Eq. (409), the matrix elements are very similar to those for the stellar atmosphere case, the only difference is the replacement $\sigma_R T_{\text{eff}}^4$ by $\sigma_R T_{\text{eff}}^4 (1 - \theta_d)$, which enters only the right-hand side vector (namely, its differential equation part). There are several additional terms in the integral equation part which we summarize below,

$$
\begin{align}
(A_d)_{NR,NH}^{\text{add}} &= \alpha_d E_0 w_d \, \mu m_H, \tag{465}\\
(B_d)_{NR,NH}^{\text{add}} &= -\alpha_d E_0 w_d \, \mu m_H, \tag{466}\\
(L_d)_{NR}^{\text{add}} &= -\alpha_d E_0 w_d \, \rho_d, \tag{467}
\end{align}
$$

where

$$E_0 = E_{\text{diss}}/\rho w = \frac{9}{16\pi} \frac{GM}{R^3} \left(\frac{A}{B}\right)^2, \tag{468}$$

as follows from Eq. (60).

Equation for vertical distance

Matrix elements for $d < ND$ are

$$
\begin{align}
(B_d)_{NZ,NH} &= \mu m_H (m_{d+1} - m_d)/2\rho_d^2, \tag{469}\\
(C_d)_{NZ,NH} &= -\mu m_H (m_{d+1} - m_d)/2\rho_{d+1}^2, \tag{470}\\
(B_d)_{NZ,NP} &= -\mu m_H (m_{d+1} - m_d)/2\rho_d^2, \tag{471}\\
(C_d)_{NZ,NP} &= \mu m_H (m_{d+1} - m_d)/2\rho_{d+1}^2, \tag{472}\\
(B_d)_{NZ,NZ} &= (C_d)_{NZ,NZ} = 1, \tag{473}\\
(L_d)_{NZ} &= z_{d+1} - z_d + \frac{m_{d+1} - m_d}{2}\left(\frac{1}{\rho_d} + \frac{1}{\rho_{d+1}}\right), \tag{474}
\end{align}
$$

and for $d = ND$ they are simply

$$(B_d)_{NZ,NZ} = 1, \quad (L_d)_{NZ} = 0. \tag{475}$$

C3. Compton scattering

Within the present setup, Compton scattering can only be treated using the traditional full complete linearization approach, because using the hybrid CL/ALI scheme is very unstable, and the Rybicki scheme cannot be easily generalized to this case while preserving its favorable numerical properties.

Here we summarize the additional terms in matrices $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, and in the right-hand side vector $\mathbf{L}$, described above in Appendix C.1. We denote these additional terms with superscript "compt".

• Matrix elements corresponding to the transfer equation: For the highest frequency, which in the linearization has index $i = 1$,

$$(B_d)^{\text{compt}}_{ii} = \mathcal{B}_i, \tag{476}$$

$$(B_d)^{\text{compt}}_{i,i+1} = \mathcal{C}_i, \tag{477}$$

$$(L_d)^{\text{compt}}_i = -\mathcal{B}_i J_i - \mathcal{C}_i J_{i+1}. \tag{478}$$

For other frequencies, one has

$$(B_d)^{\text{compt}}_{i,i-1} = \mathcal{A}_i, \tag{479}$$

$$(B_d)^{\text{compt}}_{ij} = \mathcal{B}_i, \tag{480}$$

$$(B_d)^{\text{compt}}_{i,i+1} = \mathcal{C}_i, \tag{481}$$

$$\begin{aligned}(B_d)^{\text{compt}}_{i,NR} = {} & [(-3c^-_i + d^-_i)J_{i-1} + (-3c^0_i + d^0_i)J_i \\ & + (-3c^+_i + d^+_i)J_{i+1}](n_{\text{e}}\sigma_{\text{e}}/\chi_i)(\Theta/T)\end{aligned} \tag{482}$$

$$(B_d)^{\text{compt}}_{i,NP} = S^{\text{compt}}/n_{\text{e}}, \tag{483}$$

$$(L_d)^{\text{compt}}_i = -S_{\text{compt}}. \tag{484}$$

with

$$S^{\text{compt}} = \mathcal{A}_i J_{i-1} + \mathcal{B}_i J_i + \mathcal{C}_i J_{i+1}, \tag{485}$$

• Matrix elements corresponding to the radiative equilibrium equation:

$$(B_d)^{\text{compt}}_{NR,i} = -\alpha_d \chi_{di} w_i (\mathcal{A}_{i+1} + \mathcal{B}_i + \mathcal{C}_{i-1}) \tag{486}$$

$$\begin{aligned}(B_d)^{\text{compt}}_{NR,NR} = {} & -\alpha_d \chi_{di} w_i [(-3c^-_i + d^-_i)J_{i-1} + (-3c^0_i + d^0_i)J_i \\ & + (-3c^+_i + d^+_i)J_{i+1}](n_{\text{e}}\sigma_{\text{e}}/\chi_i)(\Theta/T)\end{aligned} \tag{487}$$

$$(B_d)^{\text{compt}}_{NR,NP} = -\alpha_d \chi_{di} w_i S^{\text{compt}}/n_{\text{e}}, \tag{488}$$

$$(L_d)^{\text{compt}}_{NR} = \alpha_d \chi_{di} w_i S_{\text{compt}}. \tag{489}$$

It turns out that in some cases the overall linearization scheme is more stable if one does not linearize the Compton terms in the radiative equilibrium, so the above additional matrix elements $(B_d)_{NR,k}, k = 1, \ldots, NP$, are set to zero if needed.

Appendix D. Details of the implementation of the hybrid CL/ALI method

As shown in §3.2, the method does not linearize the mean intensity of radiation in all frequency points, but only in selected few frequencies, call "explicit"

frequencies. For the remaining frequency points, called "ALI frequencies", the mean intensity is expressed as

$$J_{dj} = \Lambda^*_{d,j}(\eta_{dj}/\kappa_{dj}) + \Delta J_{dj}. \tag{490}$$

The mean intensity in the ALI frequencies are thus removed form the state vector. The parameter NF now refers to the number of explicit frequencies.

Although TLUSTY allows for both a diagonal as well as tri-diagonal operator, here we consider a diagonal Λ^* for simplicity. In any case, numerical experience showed that although an application of the tridiagonal operator speeds up the convergence of the iterations, a similar or even faster convergence is obtained with a diagonal operator applied together with the Ng acceleration.

In the expressions for the elements of the Jacobian, the mean intensity in the ALI frequency point i is then viewed as a function of T, $n_{\rm e}$, and the set of atomic level populations $n_i, i = 1, \ldots, NL$. Denoting $x \equiv \{T, n_{\rm e}, n_i\}$, the corresponding derivatives are given by

$$\frac{\partial J_{di}}{\partial x_d} \equiv D^x_{dj} = \Lambda^*_{dj} \frac{\eta_{dj}}{\kappa_{dj}} \left(\frac{1}{\eta_{dj}} \frac{\partial \eta_{dj}}{\partial x} - \frac{1}{\kappa_{dj}} \frac{\partial \kappa_{dj}}{\partial x} \right), \tag{491}$$

where the term ΔJ_{id} is known from the previous iteration and is therefore independent of x, and consequently does not appear in linearized equations.

The elements of matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ are then modified as follows. All the expressions for the first NF rows are valid, provided that NF now refers to the number of explicit (linearized) frequency points. Analogously, the expression for the first NF columns are also unchanged. Other elements will contain additional terms that correspond to the contribution of the ALI frequencies. We will summarize the additional terms below.

We use the following notation. As specified above, x may mean any of the state vector parameters T, $n_{\rm e}$, and $n_i, i = 1, NL$. The corresponding index is denoted as NX; i.e. $NX = NR$ for $x = T$, $NX = NP$ for $x = n_{\rm e}$, etc. The total number of the ALI frequency points is denoted by NFA.

For the row corresponding to the hydrostatic equilibrium equation one has the following additional terms, denoted with superscript "ALI" ,

$$(B_1)^{\rm ALI}_{NH,NX} = (4\pi/c) \sum_{j=1}^{NFA} w_j g_j \left[\omega_{1j} D^x_{1j} + (\partial \omega_{1j}/\partial x_1) J_{1j} \right], \tag{492}$$

$$(L_1)^{\rm ALI}_{NH} = -(4\pi/c) \sum_{j=1}^{NFA} w_j \omega_{1j} g_j J_{1j}, \tag{493}$$

for the upper boundary condition, and, for $d > 1$,

$$(A_d)^{\rm ALI}_{NH,NX} = (4\pi/c) \sum_{j=1}^{NFA} w_j f_{d-1,j} D^x_{d-1,j} \tag{494}$$

$$(B_d)^{\text{ALI}}_{NH,NX} = (4\pi/c) \sum_{j=1}^{NFA} w_j f_{dj} D^x_{dj}, \tag{495}$$

$$(L_d)^{\text{ALI}}_{NH} = -(4\pi/c) \sum_{j=1}^{NFA} w_j (f_{dj} J_{dj} - f_{d-1,j} J_{d-1,j}). \tag{496}$$

For the row corresponding to the radiative equilibrium, one has the following additions.

$$(A_d)^{\text{ALI}}_{NR,NX} = \beta_d \sum_{j=1}^{NFA} w_j f_{d-1,j} D^x_{d-1,j} / \Delta\tau_{d-1/2,j}, \tag{497}$$

$$(B_d)^{\text{ALI}}_{NR,NX} = \alpha_d \sum_{j=1}^{NFA} w_j \left[\kappa_{dj} D^x_{dj} + \frac{\partial \kappa_{dj}}{\partial x_d} J_{dj} - \frac{\partial \eta_{dj}}{\partial x_d} \right]$$

$$+ \beta_d \sum_{j=1}^{NFA} w_j f_{dj} D^x_{dj} / \Delta\tau_{d-1/2,j}, \tag{498}$$

$$(L_d)^{\text{ALI}}_{NR} = -\alpha_d \sum_{j=1}^{NFA} w_j (\kappa_{dj} J_{dj} - \eta_{dj})$$

$$- \beta_d \sum_{j=1}^{NFA} w_j \frac{f_{dj} J_{dj} - f_{d-1,j} J_{d-1,j}}{\Delta\tau_{d-1/2,j}} \tag{499}$$

The set of kinetic equilibrium equations is written in the form

$$\mathbf{n} - \mathcal{A}^{-1} \cdot \mathbf{b} = 0, \tag{500}$$

from which one obtains

$$(\partial\mathbf{n}/\partial x) = -\mathcal{A}^{-1} \cdot \mathbf{V}_x. \tag{501}$$

Vector $\mathbf{V}$ represents the column of the Jacobi matrix corresponding to quantity x; x stands for any quantity of vector ψ, including linearized mean intensities.

$$\mathbf{V}_x = (\partial\mathcal{A}/\partial x) \cdot \mathbf{n} - (\partial\mathbf{b}/\partial x). \tag{502}$$

Let the transition $l \leftrightarrow u$ be represented by an arbitrary combination of the "explicit" and "ALI" frequency points; either subset is allowed to be empty. Generally, the contribution from this transition comes only to the two following components of vector $\mathbf{V}_x$, namely

$$(\mathbf{V}_x)_l = \frac{\partial(R_{lu} + C_{lu})}{\partial x} n_l - \frac{\partial(R_{ul} + C_{ul})}{\partial x} n_u,$$

$$(\mathbf{V}_x)_u = -(\mathbf{V}_x)_l. \tag{503}$$

The radiative rate is written in a discretized form as

$$R_{lu} = (4\pi/h) \left[\sum_{i=1}^{NF} w_i \sigma_{lu}(\nu_i) J_i / \nu_i + \sum_{j=1}^{NFA} w_j \sigma_{lu}(\nu_j) J_j / \nu_j, \right], \tag{504}$$

and similarly for the downward rate. The contribution to $\mathbf{V}_x$ from the collisional rates and from the "explicit" frequency points is the same as in the case of the standard CL, whereas the ALI contribution is given by

$$(V_x)_l^{\mathrm{ALI}} = [n_l - n_u G_{lu}(\nu)](4\pi/h) \sum_{j=1}^{NFA} w_j \sigma_{lu}(\nu_j) D_j^x / \nu_j, \qquad (505)$$

where D_j^x is given by equation (491). The important differences from the standard complete linearization is that because the derivatives D_j^x are generally nonzero for x being the individual level populations, the Jacobian contains contributions from the populations. This of course expresses the fact stated already that within the ALI formalism the kinetic equilibrium equations are nonlinear in the level populations.

The charge conservation equation, and the additional terms for convection are independent of the radiation field, and therefore are the same as in the traditional complete linearization.

Appendix E. Implementation of the Rybicki scheme

The overall structure of the global Jacobian is reversed from the original complete linearization, in the sense that the role of frequencies and depths is reversed. Although one may use the idea of the hybrid CL/ALI method, in the sense that only some frequency points are taken as explicit, it is not very practical because it slows down the convergence rate of the linearization iteration. Therefore, all the frequency points are taken as explicit. For convenience, we repeat here the basic equations of both schemes.

For complete linearization

$$-\mathbf{A}_d \delta\psi_{d-1} + \mathbf{B}_d \delta\psi_d - \mathbf{C}_d \delta\psi_{d+1} = \mathbf{L}_d, \qquad (506)$$

where
$$\psi_d = \{J_1, \ldots, J_{NF}, N, T, n_{\mathrm{e}}, n_1, \ldots, n_{NL}, [n_m], [\nabla], [z]\}. \qquad (507)$$

Here, A, B, and C are $NN \times NN$ matrices, and L is a residual error vector.

For the Rybicki scheme,

$$\mathbf{U}_i \delta\mathbf{J}_i + \mathbf{R}_i \delta\mathbf{T} = \mathbf{E}, \qquad (508)$$

with
$$\delta\mathbf{J}_i \equiv \{\delta J_{1i}, \delta J_{2i}, \ldots, \delta J_{ND,i}\}, \quad i = 1, \ldots, NF, \qquad (509)$$

and
$$\delta\mathbf{T} \equiv \{\delta T_1, \delta T_2, \ldots, \delta T_{ND}\}. \qquad (510)$$

Here, the only state parameter besides the mean intensities is the temperature. Therefore, one has to view all the other state parameters as functions of

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T. Consequently, instead of employing the partial derivatives $\partial\chi/\partial T$, $\partial\chi/\partial n_{\rm e}$, $\partial\chi/\partial n_i$, etc., one has to consider a total derivative $D\chi/DT$, and analogously for the derivatives of the emission and scattering coefficients,

The components corresponding to the radiative transfer equation are the following. The tridiagonal matrices $\mathbf{U}$ that contain derivatives with respect to the mean intensities are exactly analogous to the corresponding elements of matrices $\mathbf{A}$, $\mathbf{B}$, and $\mathbf{C}$ of complete linearization,

$$U_{dd,i} = (B_d)_{ii}, \quad U_{d,d-1,i} = (A_d)_{ii}, \quad U_{d,d+1,i} = (C_d)_{ii}. \tag{511}$$

Components of matrices $\mathbf{R}$ are similar, but not identical, to the components of the original matrices,

$$R_{dd,i} = (B_d)_{i,NR}, \quad R_{d,d-1,i} = (A_d)_{i,NR}, \tag{512}$$

where we replace the partial derivatives $\partial\chi/\partial T$, $\partial\eta/\partial T$, $\partial\sigma/\partial T$ by the total derivatives $D\chi/DT$, $D\eta/DT$, and $D\sigma/DT$, respectively. The right-hand side vector is given by

$$E_{d,i} = (L_d)_i. \tag{513}$$

Similarly, for the radiative equilibrium equation,

$$V_{dd,i} = (B_d)_{NR,i}, \quad V_{d,d-1,i} \equiv (A_d)_{NR,i}, \tag{514}$$

$$W_{dd,i} = (B_d)_{NR,NR}, \quad W_{d,d-1,i} = (A_d)_{NR,NR}, \tag{515}$$

$$F_d = (L_d)_{NR}, \tag{516}$$

where again in Eq. (515) one replaces $\partial\kappa/\partial T$ and $\partial\eta/\partial T$ by $D\kappa/DT$ and $D\eta/DT$.

The total derivatives are computed numerically as, for instance for χ,

$$\frac{D\chi_d}{DT_d} = \frac{\widetilde{\chi}_d - \chi_d}{\Delta T_d}, \tag{517}$$

where ΔT_d is set to $0.01T_d$. We denote the new temperature $T_d + \Delta T_d$ as $\widetilde{T}_d$. The corresponding $\widetilde{\chi}_d$ is computed by the following multi-step procedure:

(i) Update of the gas pressure, denoted here as $\widetilde{P}$, by solving the hydrostatic equilibrium equation,

$$\widetilde{P}_1 = m_1(g - g_1^{\rm rad}), \tag{518}$$

$$\widetilde{P}_d = \widetilde{P}_{d-1} + (m_d - m_{d-1})\left[g - g_d^{\rm rad}(1 + 4\Delta T_d)\right], \quad d > 1, \tag{519}$$

where

$$g_1^{\rm rad} = (4\pi/c\rho_1)\sum_{i=1}^{NF} w_i\chi_{1i}g_iJ_{1i}, \tag{520}$$

$$g_d^{\rm rad} = (4\pi/c)\sum_{i=1}^{NF} w_i\frac{f_{di}J_{di} - f_{d-1,i}J_{d-1,i}}{m_d - m_{d-1}}, \quad d > 1 \tag{521}$$

is the current value of the radiation acceleration. The last term in Eq. (519) represents an approximate modification of the radiation pressure due to modified temperature by expressing $P^{\mathrm{rad}} = \gamma P^{\mathrm{rad,TE}} \propto \gamma T^4$, (with the superscript "TE" denoting the thermodynamic equilibrium), and thus

$$P^{\mathrm{rad}}(T + \Delta T) \approx P^{\mathrm{rad}}(T) + (dP^{\mathrm{rad}}/dT)\Delta T = P^{\mathrm{rad}}(1 + 4\Delta T), \qquad (522)$$

which assumes that the non-equilibrium proportionality parameter γ remains unchanged, and that the radiation pressure varies slowly with depth so that the same thermodynamic relation can be used also for the radiation acceleration.

(ii) Compute new total particle density for the new gas pressure,

$$\widetilde{N}_d = \widetilde{P}_d/(k\widetilde{T}_d). \qquad (523)$$

(iii) For the new $\widetilde{N}_d$, compute the new electron number density $\widetilde{n}_{\mathrm{e}}$ by solving a set of Saha equations and the charge conservation equation.

(iv) Using the new $\widetilde{T}$ and $\widetilde{n}_{\mathrm{e}}$, and using current values of the radiative rates and collisional cross sections, solve the set of kinetic equilibrium equations to obtain a new set of populations $\widetilde{n}_i, i = 1, \ldots, NL$. Notice that in the case of LTE the kinetic equilibrium equations are replaced by the set of Saha-Boltzmann expression for the level populations.

(v) Finally, the opacities and emissivities are evaluated by standard expressions for the new values of $\widetilde{T}$, $\widetilde{n}_{\mathrm{e}}$, and $\widetilde{n}_i$,

$$\widetilde{\chi}_d = \chi_d(\widetilde{T}, \widetilde{n}_{\mathrm{e}}, \{\widetilde{n}_i\}), \qquad (524)$$

and analogously for η and σ.

Appendix F. Partial frequency redistribution

This process is not a main emphasis of TLUSTY, but can be included in an approximate way. In the present version of TLUSTY, only the H I Lyman α, the Mg I resonance line at $\lambda 2852$ Å, and the Mg II resonance lines at $\lambda\lambda 2796, 2803$ Å can be treated with partial redistribution, namely using the partial coherent scattering approximation.

Under the usual approximation of *complete frequency redistribution* (CFR), there is no correlation between the frequencies of an absorbed and an emitted photon during the process of resonance scattering in a line, that is a radiative transition from level i to level j, immediately followed by a radiative transition from j to i.

A more general approach is called the *partial frequency redistribution* (PFR, but often, and in the past, an acronym PRD was used). In this case, there is a correlation between the absorbed and emitted photons described through the *redistribution function*. For a comprehensive discussion refer to Hubeny & Mihalas (2014; Chaps.10 and 15). The most appropriate redistribution function

for a resonance line is a linear combination of complete redistribution, and coherent scattering on the atom's frame, which in the observer's frame is described through the redistribution function R_{II}. The latter can further be approximated by another linear combination of complete redistribution and coherent scattering in the laboratory frame, called *partial coherent scattering approximation* [Jefferies & White (1960), Kneer (1975), Hubeny & Mihalas (2014, § 15.3)].

The presence of PFR effects changes in principle both the emission coefficient in the line, as well as the radiative rates. As discussed for instance in Hubeny & Mihalas (2014, § 15.1), the latter effects are usually very small, so in TLUSTY only a modification of the emission coefficient is taken into account. One makes another approximation that the effects of partial redistribution are negligible in the line core, which further simplifies the modifications needed to treat the PFR effects in TLUSTY.

For a line chosen to be with PFR, the emission coefficient for the ordinary complete redistribution is given by, neglecting stimulated emission,

$$\eta_{ij}^{\mathrm{CFR}}(x) = n_j A_{ji} \phi_{ij}(x), \tag{525}$$

where $x = (\nu - \nu_0)/\Delta\nu_D$ is the frequency difference from the liner center expressed in units of Doppler width, A_{ji} is the Einstein coefficient for spontaneous emission from level j to i, and $\phi(x)$ is the (normalized) absorption profile coefficient that expresses the frequency dependence of the line absorption cross section, typically given by a Voigt profile, or a special profile in the case of hydrogen.

The approximate treatment of PFR adopted in TLUSTY consists of two simple modifications of the standard CFR approach: The modifications for the approximate approach adopted in TLUSTY is:

(i) Replacing the emission coefficient with

$$\eta_{ij}^{\mathrm{PFR}}(x) = \eta_{ij}^{\mathrm{CFR}}(x)[1 - \gamma_{ij}\bar{s}(x)], \tag{526}$$

where $\bar{s}(x)$ is a step function, $\bar{s}(x) = 0$ for $x \leq x_{\mathrm{div}}$, and $\bar{s}(x) = 1$ for $> x_{\mathrm{div}}$; and x_{div} is the so-called *division frequency*, which is an input parameter (XPDIV). γ is the so-called *coherence fraction*, given approximately by,

$$\gamma_{ij} \approx A_{ji}/\Gamma_{ij}, \tag{527}$$

where Γ_{ij} is the line broadening parameter [see Eq. (99)]. The simple form of Eq. (527) follows from neglecting various other processes, such as inelastic collisions.

(ii) Adding a coherent scattering term to the original scattering terms, which is usually just the electron (Thomson) scattering,

$$\sigma(\nu) = \sigma^{\mathrm{orig}}(\nu) + \kappa_{ij}(\nu)\gamma_{ij}\bar{s}(x). \tag{528}$$

The above treatment of partial redistribution is admittedly very crude, but it should be kept in mind that this approach is designed only to assess possible

modifications of the global atmospheric structure due to PFR in some lines, which, in the vast majority of cases, is relatively small. To compute detailed line profiles with more accurate treatment of PFR, one can always take an atmospheric structure computed by TLUSTY and use it in another codes specifically designed to produce line profiles with a more sophisticated treatment of PFR.

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