New Escape Probabilities for ProDiMo

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The currently used escape probability method in ProDiMo, which enters the non-LTE rate equations and the calculation of the line heating/cooling rates, is based on Eq. (73) in Woitke et al. (2009), which is a rather crude approximation as it only considers radiative pumping by continuum photons in the radial direction, and line photon escape into the upward vertical direction. In particular, the IR-pumping from the disc below is incorrectly attenuated by the radial line optical depth $\tau_{ul}^{\rm rad}$, which can be huge, i.e. we are likely underestimating the true IR pumping. In addition, in the outer optically thin disc regions, the escape probability is currently limited to $P_{ul}^{\rm esc} \le \frac{1}{2}$, where it should be $P_{ul}^{\rm esc} \to 1$.

This document presents a new idea how to calculate the line averaged mean intensity ("J-bar") more rigorously by taking into account continuum radiative transfer effects in the resonance region

$$\bar{J}_{ul} = \frac{1}{4\pi} \iint \phi_\nu \, I_\nu(\vec{n}) \, d\Omega \, d\nu \ , \tag{1}$$

where ϕ_ν is the line profile function associated with the spectral line $u \to l$ and I_ν is the spectral intensity. We will show that, by making some assumptions about disk geometry and locality of radiative transfer quantities explained below, it is possible to arrive at a final expression that reads again

$$\bar{J}_{ul} = P_{ul}^{\rm pump} J_\nu^{\rm cont} + (1 - P_{ul}^{\rm esc}) S_{\rm L} \tag{2}$$

but now with new $P_{ul}^{\rm pump}$ and $P_{ul}^{\rm esc}$ that depend not only on line optical depths, but also on continuum optical depths, and take into account pumping from and escape into all directions. $S_{\rm L}$ is the line source function and $J_\nu^{\rm cont}$ the continuous mean intensity that would result if the line has zero opacity.

1 The new escape probability method

We write the line & continuum radiative transfer equation as

$$\frac{dI_\nu}{ds} = -(\kappa_{\rm C} + \kappa_{\rm L}\phi_\nu) I_\nu \ + \ \kappa_{\rm C} S_{\rm C} \ + \ \kappa_{\rm L}\phi_\nu S_{\rm L} \tag{3}$$

where the continuum, absorption and scattering opacities [cm^{-1}], and the continuum source function, assuming isotropic scattering, are given by

$$\kappa_{\rm C} \ = \ \kappa_\nu^{\rm abs} + \kappa_\nu^{\rm sca} \ , \tag{4}$$

$$\kappa_{\rm C}\, S_{\rm C} \ = \ \kappa_\nu^{\rm abs} B_\nu(T_{\rm dust}) + \kappa_\nu^{\rm sca} J_\nu^{\rm cont} \ . \tag{5}$$

The line opacity [cm^{-1} Hz], Gaussian line profile function [Hz^{-1}], and line source function [erg cm^{-2} s^{-1} Hz^{-1} sr^{-1}] are given by

$$\kappa_{\rm L} \ = \ \frac{h\nu_{ul}}{4\pi} \big(n_l B_{lu} - n_u B_{ul} \big) \ , \tag{6}$$

$$\phi_\nu \ = \ \frac{1}{\sqrt{\pi}\Delta\nu_{\rm D}} \, {\rm e}^{-\left(\frac{\nu-\nu_{ul}}{\Delta\nu_{\rm D}}\right)^2} \ , \tag{7}$$

$$S_{\rm L} \ = \ \frac{2h\nu_{ul}^3}{c^2} \left(\frac{g_u\, n_l}{g_l\, n_u} - 1 \right)^{-1} \ , \tag{8}$$

where ν_{ul} is the line centre frequency, $\nu_{\rm D} = \nu_{ul}\,\Delta v/c$ the Doppler width and $\Delta v = \sqrt{v_{\rm th}^2 + v_{\rm turb}^2}$ the line width in velocity space. Introducing the optical depth and maximum optical depth as

$$t_\nu(s) = \int_0^s \kappa_{\rm C} + \kappa_{\rm L}\phi_\nu\,ds \ , \tag{9}$$

$$\tau_\nu = t_\nu(s_{\rm max}) \ , \tag{10}$$

the formal solution of Eq. (3) is

$$I_\nu(\vec{n}) = I^0_\nu(\vec{n})\,{\rm e}^{-\tau_\nu} + \int_0^{s_{\rm max}} (\kappa_{\rm C}S_{\rm C} + \kappa_{\rm L}\phi_\nu S_{\rm L})\,{\rm e}^{-t_\nu}\,ds \ , \tag{11}$$

where $\vec{n}$ is the direction of the ray (unit vector) and $s_{\rm max}$ is the distance backward along the ray up to the point where the ray enters the model volume. $I^0_\nu(\vec{n})$ is the incident intensity at that point in direction $\vec{n}$.

Assumption 1 (locality): We assume that all radiative transfer properties, that is $\kappa_{\rm C}$, $\kappa_{\rm L}$, $S_{\rm L}$, $S_{\rm C}$ and ϕ_ν, are independent of location and direction, and given by their local values. Assuming $S_{\rm L} = $ const is standard in escape probability theory, because the line photons typically interact only within a small "resonance volume" around the point of interest. Generalising this idea to the continuum transfer properties is a new idea Hummer & Rybicki (however, see 1985).

This way, we try to capture the most relevant continuum radiative transfer effects in that resonance region, where there is a competition between line and continuum photons. Constant ϕ_ν also means that we neglect velocity line shifts, i.e. we assume a static medium. The only quantities that are allowed to depend on direction are $I^0_\nu(\vec{n})$ and $s_{\rm max}$ (and hence τ_ν). In this case the formal solution of the RT equation (11) simplifies to

$$I_\nu(\vec{n}) = I^0_\nu(\vec{n})\,{\rm e}^{-\tau_{\rm C}-\tau_{\rm L}\phi_\nu} + \frac{\tau_{\rm C}S_{\rm C} + \tau_{\rm L}\phi_\nu S_{\rm L}}{\tau_{\rm C} + \tau_{\rm L}\phi_\nu}\Big(1 - {\rm e}^{-\tau_{\rm C}-\tau_{\rm L}\phi_\nu}\Big) \ , \tag{12}$$

where we have used the continuum and line centre optical depths $\tau_{\rm C} = \kappa_{\rm C}s_{\rm max}$ and $\tau_{\rm L} = \kappa_{\rm L}s_{\rm max}$.

Assumption 2 (disc geometry): We consider three major directions: radial (the rays coming from the stellar surface – often important for pumping), vertically upwards and vertically downwards. At a given location in the disc, the star occupies a small solid angle $\Omega_\star$. The other two principle directions cover half of $\Omega_{\rm d} = 4\pi - \Omega_\star$ each. All rays coming from the stellar surface are represented by a single radial ray. For the upward and downward directions, we approximate the disk as being plane-parallel with $\mu = \cos(\theta)$ where θ is the angle with the vertical. Thus we find from Eq. (1)

$$\bar{J}_{ul} = \frac{\Omega_\star}{4\pi}\int \phi_\nu\,I^{\rm rad}_\nu\,d\nu + \frac{\Omega_{\rm d}}{8\pi}\int \phi_\nu \int_0^1 I_\nu(\mu)\,d\mu\,d\nu + \frac{\Omega_{\rm d}}{8\pi}\int \phi_\nu \int_{-1}^0 I_\nu(\mu)\,d\mu\,d\nu \ . \tag{13}$$

Introducing the vertically upwards and downwards (accross the disc) line and continuum optical depths, $\tau^\uparrow_{\rm L}$, $\tau^\downarrow_{\rm L}$, $\tau^\uparrow_{\rm C}$ and $\tau^\downarrow_{\rm C}$, respectively, and the radially inward line and continuum optical depths, $\tau^{\rm rad}_{\rm L}$ and $\tau^{\rm rad}_{\rm C}$, and using plane-parallel geometry $\tau(\mu) = \tau(\mu = 0)/\mu$ we obtain from Eqs. (12) and (13)

$$\bar{J}_{ul} = \frac{\Omega_\star}{4\pi}\int \phi_\nu \left(I^\star_\nu\,{\rm e}^{-\tau^{\rm rad}_{\rm C}-\tau^{\rm rad}_{\rm L}\phi_\nu} + \frac{\tau^{\rm rad}_{\rm C}S_{\rm C} + \tau^{\rm rad}_{\rm L}\phi_\nu S_{\rm L}}{\tau^{\rm rad}_{\rm C} + \tau^{\rm rad}_{\rm L}\phi_\nu}\Big(1 - {\rm e}^{-\tau^{\rm rad}_{\rm C}-\tau^{\rm rad}_{\rm L}\phi_\nu}\Big)\right) d\nu \tag{14}$$

$$+ \frac{\Omega_{\rm d}}{8\pi}\int \phi_\nu \int_0^1 I^{\rm ISM}_\nu\,{\rm e}^{-\frac{\tau^\uparrow_{\rm C}}{\mu}-\frac{\tau^\uparrow_{\rm L}}{\mu}\phi_\nu} + \frac{\tau^\uparrow_{\rm C}S_{\rm C} + \tau^\uparrow_{\rm L}\phi_\nu S_{\rm L}}{\tau^\uparrow_{\rm C} + \tau^\uparrow_{\rm L}\phi_\nu}\left(1 - {\rm e}^{-\frac{\tau^\uparrow_{\rm C}}{\mu}-\frac{\tau^\uparrow_{\rm L}}{\mu}\phi_\nu}\right) d\mu\,d\nu \tag{15}$$

$$+ \frac{\Omega_{\rm d}}{8\pi}\int \phi_\nu \int_{-1}^0 I^{\rm ISM}_\nu\,{\rm e}^{-\frac{\tau^\downarrow_{\rm C}}{|\mu|}-\frac{\tau^\downarrow_{\rm L}}{|\mu|}\phi_\nu} + \frac{\tau^\downarrow_{\rm C}S_{\rm C} + \tau^\downarrow_{\rm L}\phi_\nu S_{\rm L}}{\tau^\downarrow_{\rm C} + \tau^\downarrow_{\rm L}\phi_\nu}\left(1 - {\rm e}^{-\frac{\tau^\downarrow_{\rm C}}{|\mu|}-\frac{\tau^\downarrow_{\rm L}}{|\mu|}\phi_\nu}\right) d\mu\,d\nu \ . \tag{16}$$

Introducing the second exponential integral function $E_2(\tau)=\int_0^1 \exp\big(-\frac{\tau}{\mu}\big)\,d\mu$ we find

$$\begin{aligned}
\bar{J}_{ul} &= \frac{\Omega_\star}{4\pi}\int \phi_\nu\left(I_\nu^\star\,\mathrm{e}^{-\tau_\mathrm{C}^\mathrm{rad}-\tau_\mathrm{L}^\mathrm{rad}\phi_\nu}+\frac{\tau_\mathrm{C}^\mathrm{rad}S_\mathrm{C}+\tau_\mathrm{L}^\mathrm{rad}\phi_\nu S_\mathrm{L}}{\tau_\mathrm{C}^\mathrm{rad}+\tau_\mathrm{L}^\mathrm{rad}\phi_\nu}\Big(1-\mathrm{e}^{-\tau_\mathrm{C}^\mathrm{rad}-\tau_\mathrm{L}^\mathrm{rad}\phi_\nu}\Big)\right)d\nu \qquad (17)\\
&+ \frac{\Omega_\mathrm{d}}{8\pi}\int \phi_\nu\left(I_\nu^\mathrm{ISM}\,E_2(\tau_\mathrm{C}^\uparrow+\tau_\mathrm{L}^\uparrow\phi_\nu)+\frac{\tau_\mathrm{C}^\uparrow S_\mathrm{C}+\tau_\mathrm{L}^\uparrow\phi_\nu S_\mathrm{L}}{\tau_\mathrm{C}^\uparrow+\tau_\mathrm{L}^\uparrow\phi_\nu}\Big(1-E_2(\tau_\mathrm{C}^\uparrow+\tau_\mathrm{L}^\uparrow\phi_\nu)\Big)\right)d\nu \qquad (18)\\
&+ \frac{\Omega_\mathrm{d}}{8\pi}\int \phi_\nu\left(I_\nu^\mathrm{ISM}\,E_2(\tau_\mathrm{C}^\downarrow+\tau_\mathrm{L}^\downarrow\phi_\nu)+\frac{\tau_\mathrm{C}^\downarrow S_\mathrm{C}+\tau_\mathrm{L}^\downarrow\phi_\nu S_\mathrm{L}}{\tau_\mathrm{C}^\downarrow+\tau_\mathrm{L}^\downarrow\phi_\nu}\Big(1-E_2(\tau_\mathrm{C}^\downarrow+\tau_\mathrm{L}^\downarrow\phi_\nu)\Big)\right)d\nu\ , \qquad (19)
\end{aligned}$$

where $I_\nu^\star$ and I_ν^ISM are the stellar and interstellar incident intensities, respectively. We now introduce the dimensionless profile function $\phi(x)=\exp(-x^2)/\sqrt{\pi}$ with $x=(\nu-\nu_{ul})/\Delta\nu_\mathrm{D}$ and six basic 2D-functions, which all produce values between 0 and 1, to further simplify the result

$$\begin{aligned}
\alpha_0(\tau_\mathrm{L},\tau_\mathrm{C}) &= \int \phi(x)\,\mathrm{e}^{-\tau_\mathrm{C}-\tau_\mathrm{L}\phi(x)}\,dx\ , \qquad (20)\\
\alpha_1(\tau_\mathrm{L},\tau_\mathrm{C}) &= \int \phi(x)\,\frac{\tau_\mathrm{C}}{\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)}\big(1-\mathrm{e}^{-\tau_\mathrm{C}-\tau_\mathrm{L}\phi(x)}\big)\,dx\ , \qquad (21)\\
\alpha_2(\tau_\mathrm{L},\tau_\mathrm{C}) &= \int \phi(x)\,\frac{\tau_\mathrm{L}\phi(x)}{\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)}\big(1-\mathrm{e}^{-\tau_\mathrm{C}-\tau_\mathrm{L}\phi(x)}\big)\,dx\ , \qquad (22)\\
\beta_0(\tau_\mathrm{L},\tau_\mathrm{C}) &= \int \phi(x)\,E_2\big(\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)\big)\,dx\ , \qquad (23)\\
\beta_1(\tau_\mathrm{L},\tau_\mathrm{C}) &= \int \phi(x)\,\frac{\tau_\mathrm{C}}{\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)}\Big(1-E_2\big(\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)\big)\Big)\,dx\ , \qquad (24)\\
\beta_2(\tau_\mathrm{L},\tau_\mathrm{C}) &= \int \phi(x)\,\frac{\tau_\mathrm{L}\phi(x)}{\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)}\Big(1-E_2\big(\tau_\mathrm{C}+\tau_\mathrm{L}\phi(x)\big)\Big)\,dx\ , \qquad (25)
\end{aligned}$$

resulting in

$$\begin{aligned}
\bar{J}_{ul} &= \tfrac{\Omega_\star}{4\pi}\Big(I_\nu^\star\,\alpha_0(\tau_\mathrm{L}^\mathrm{rad},\tau_\mathrm{C}^\mathrm{rad}) + S_\mathrm{C}\,\alpha_1(\tau_\mathrm{L}^\mathrm{rad},\tau_\mathrm{C}^\mathrm{rad}) + S_\mathrm{L}\,\alpha_2(\tau_\mathrm{L}^\mathrm{rad},\tau_\mathrm{C}^\mathrm{rad})\Big)\\
&+ \tfrac{\Omega_\mathrm{d}}{8\pi}\Big(I_\nu^\mathrm{ISM}\,\beta_0(\tau_\mathrm{L}^\uparrow,\tau_\mathrm{C}^\uparrow) + S_\mathrm{C}\,\beta_1(\tau_\mathrm{L}^\uparrow,\tau_\mathrm{C}^\uparrow) + S_\mathrm{L}\,\beta_2(\tau_\mathrm{L}^\uparrow,\tau_\mathrm{C}^\uparrow)\Big) \qquad (26)\\
&+ \tfrac{\Omega_\mathrm{d}}{8\pi}\Big(I_\nu^\mathrm{ISM}\,\beta_0(\tau_\mathrm{L}^\downarrow,\tau_\mathrm{C}^\downarrow) + S_\mathrm{C}\,\beta_1(\tau_\mathrm{L}^\downarrow,\tau_\mathrm{C}^\downarrow) + S_\mathrm{L}\,\beta_2(\tau_\mathrm{L}^\downarrow,\tau_\mathrm{C}^\downarrow)\Big)\ .
\end{aligned}$$

From this geometric model we also get a prediction of the continuum, i.e. the mean intensity at line centre frequency as would be present if the line opacity was zero

$$\begin{aligned}
J_\nu^\mathrm{cont} &= \tfrac{\Omega_\star}{4\pi}\Big(I_\nu^\star\,\alpha_0(0,\tau_\mathrm{C}^\mathrm{rad}) + S_\mathrm{C}\,\alpha_1(0,\tau_\mathrm{C}^\mathrm{rad})\Big)\\
&+ \tfrac{\Omega_\mathrm{d}}{8\pi}\Big(I_\nu^\mathrm{ISM}\,\beta_0(0,\tau_\mathrm{C}^\uparrow) + S_\mathrm{C}\,\beta_1(0,\tau_\mathrm{C}^\uparrow)\Big) \qquad (27)\\
&+ \tfrac{\Omega_\mathrm{d}}{8\pi}\Big(I_\nu^\mathrm{ISM}\,\beta_0(0,\tau_\mathrm{C}^\downarrow) + S_\mathrm{C}\,\beta_1(0,\tau_\mathrm{C}^\downarrow)\Big)\ .
\end{aligned}$$

Equation (27) is used to determine S_C. This means that we can calibrate S_C in such a way that our simple 3-way RT model with constant quantities results in the correct J_ν^cont as known from the proper solution of the continuum ratiave transfer problem. This is a great advantage as it allows us to eliminate most the principle problems coming with that simplified 3-way RT model in the continuum.

Comparing Eq. (26) to Eq. (2) we find the definitions of our new pumping and escape probabilities

$$P_{ul}^{\rm pump} = \frac{1}{J_\nu^{\rm cont}}\Bigg(\frac{\Omega_\star}{4\pi}\Big[I_\nu^\star\,\alpha_0(\tau_{\rm L}^{\rm rad},\tau_{\rm C}^{\rm rad}) + S_{\rm C}\,\alpha_1(\tau_{\rm L}^{\rm rad},\tau_{\rm C}^{\rm rad})\Big]$$
$$+\frac{\Omega_{\rm d}}{8\pi}\Big[I_\nu^{\rm ISM}\left(\beta_0(\tau_{\rm L}^\uparrow,\tau_{\rm C}^\uparrow)+\beta_0(\tau_{\rm L}^\downarrow,\tau_{\rm C}^\downarrow)\right) + S_{\rm C}\left(\beta_1(\tau_{\rm L}^\uparrow,\tau_{\rm C}^\uparrow)+\beta_1(\tau_{\rm L}^\downarrow,\tau_{\rm C}^\downarrow)\right)\Big]\Bigg)\ , \quad (28)$$

$$P_{ul}^{\rm esc} = 1 - \frac{\Omega_\star}{4\pi}\alpha_2(\tau_{\rm L}^{\rm rad},\tau_{\rm C}^{\rm rad}) - \frac{\Omega_{\rm d}}{8\pi}\left(\beta_2(\tau_{\rm L}^\uparrow,\tau_{\rm C}^\uparrow)+\beta_2(\tau_{\rm L}^\downarrow,\tau_{\rm C}^\downarrow)\right)\ . \quad (29)$$

2 Practical computations

In practise, the six basic 2D-functions $\alpha_0(\tau_{\rm L},\tau_{\rm C})\,...\,\beta_2(\tau_{\rm L},\tau_{\rm C})$ are precalculated and then interpolated in 2D-tables. $I_\nu^\star$ and $I_\nu^{\rm ISM}$ are known functions, and $\tau_{\rm C}^{\rm rad}$, $\tau_{\rm C}^\uparrow$ and $\tau_{\rm C}^\downarrow$ are available after the initialisation of the disk structure and opacities in ProDiMo, which allows us to determine $S_{\rm C}$ from Eq. (27) at any point and frequency. The centre line optical depths $\tau_{\rm L}^{\rm rad}$ and $\tau_{\rm L}^\uparrow$ are integrated during the downward/outward sweep of the chemistry and heating/cooling balance in ProDiMo, just as before, but we also need $\tau_{\rm L}^\downarrow$ here, which requires another assumption.

Assumption 3 (downward line optical depths): We calculate $\tau_{\rm L}^\downarrow$ by assuming that the line/continuum opacity ratio is the same for the upward and downward rays

$$\tau_{\rm L}^\downarrow = \tau_{\rm L}^\uparrow\,\frac{\tau_{\rm C}^\downarrow}{\tau_{\rm C}^\uparrow}\ . \quad (30)$$

One could try other approximations here, or use information from a previous disk iteration if required.

3 Comparison to the old escape probability method

To compare our new formalism to the old escape probability method in ProDiMo based on

$$P_{ul}^{\rm pump,old}(\tau_{\rm L}) = \int\phi(x)\,{\rm e}^{-\tau_{\rm L}\phi(x)}\,dx\ , \quad (31)$$
$$P_{ul}^{\rm esc,old}(\tau_{\rm L}) = \frac{1}{2}\int\phi(x)\,E_2\big(\tau_{\rm L}\phi(x)\big)\,dx\ , \quad (32)$$

we can identify two cases where the results are the same.

1. If the stellar illumination dominates we have

$$J_\nu^{\rm cont} = \frac{\Omega_\star}{4\pi}I_\nu^\star\,{\rm e}^{-\tau_{\rm C}^{\rm rad}}$$
$$\bar{J}_{ul} = \frac{\Omega_\star}{4\pi}I_\nu^\star\,\alpha_0(\tau_{\rm L}^{\rm rad},\tau_{\rm C}^{\rm rad}) = \frac{\Omega_\star}{4\pi}I_\nu^\star\int\phi(x)\,{\rm e}^{-\tau_{\rm C}^{\rm rad}-\tau_{\rm L}^{\rm rad}\phi(x)}\,dx = J_\nu^{\rm cont}P_{ul}^{\rm pump,old}(\tau_{\rm L}^{\rm rad})\ ,$$

   and therefore $P_{ul}^{\rm pump} = \bar{J}_{ul}/J_\nu^{\rm cont} = \alpha_0(\tau_{\rm L},\tau_{\rm C})/{\rm e}^{-\tau_{\rm C}} = P_{ul}^{\rm pump,old}(\tau_{\rm L})$ is correct in this case.

2. Considering the limiting case $\Omega_\star\to 0$, i.e. $\Omega_{\rm d}/(8\pi)=1/2$, and assuming the escape is purely vertically upward (for instance, $\tau_{\rm C}^\downarrow\to\infty$ would ensure that) we have

$$P_{ul}^{\rm esc} = 1-\frac{1}{2}\Big(\beta_2(\tau_{\rm L}^\uparrow,\tau_{\rm C}^\uparrow)\Big) = 1-\frac{1}{2}\int\phi(x)\,\frac{\tau_{\rm L}^\uparrow\phi(x)}{\tau_{\rm C}^\uparrow+\tau_{\rm L}^\uparrow\phi(x)}\,\Big(1-E_2\big(\tau_{\rm C}^\uparrow+\tau_{\rm L}^\uparrow\phi(x)\big)\Big)\,dx\ .$$

   If we now ignore the escape being hindered by the continuum (i.e. assuming $\tau_{\rm C}^\uparrow=0$) then

$$P_{ul}^{\rm esc} = 1-\frac{1}{2}\int\phi(x)\,\Big(1-E_2\big(\tau_{\rm L}^\uparrow\phi(x)\big)\Big)\,dx = \frac{1}{2}\int\phi(x)\,E_2\big(\tau_{\rm L}^\uparrow\phi(x)\big)\,dx = P_{ul}^{\rm esc,old}(\tau_{\rm L}^\uparrow)\ .$$

These two cases can be used to check the numerical implementation of the new escape probability method in ProDiMo.

Peter Woitke, October 18, 2022

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