ASTR 241 radiative transfer supplement

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1. Einstein A and B coefficients

Consider two states, u and ℓ, of an atom or molecule for which transitions between these states which are **induced by collisions with a species with number density** $\boldsymbol{n_0}$ (in cm^{-3}) are much more frequent than by any other process. Take state u to be the higher-energy one. In a steady state, transitions between the two energy levels must have the same rate: $n_u n_0 \gamma_{u\ell} = n_\ell n_0 \gamma_{\ell u}$, where the ns are number densities of the particles and the γs are collisional transition rate coefficients (in $\mathrm{cm}^3\ \mathrm{sec}^{-1}$), in general functions of temperature. So far this condition is **detailed balance in steady state**. *A priori* we know nothing about any of these quantities. If, however, the molecular region were also in thermal equilibrium at temperature T, the densities in states u and ℓ would have to be related by the Maxwell-Boltzmann distribution, $n_u/n_\ell = (g_u/g_\ell)\exp(-\Delta E_{u\ell}/kT)$, where the gs are the degeneracies of the states and $\Delta E_{u\ell}$ their energy difference. In this case,

$$g_\ell \gamma_{\ell u} = g_u \gamma_{u\ell} \exp(-\Delta E_{u\ell}/kT) = g_u \gamma_{u\ell} \exp(-h\nu/kT) \quad , \tag{1}$$

where $\nu = \nu_{u\ell}$ is the frequency of light that would be emitted in a downward radiative transition between the states. This has to be true at all temperatures, and because it is independent of densities, it has to be true at all densities as well – whether or not the molecular region is actually in thermal equilibrium. This condition is called **detailed balance in thermal equilibrium.**

Now suppose that the same species lived in a place in which radiative transitions were more frequent than any other process. In this case, steady-state detailed balance is expressed by

$$n_u A_{u\ell} + n_u B_{u\ell} U_\nu \delta\nu = n_\ell B_{\ell u} U_\nu \delta\nu \quad , \tag{2}$$

where $A_{u\ell}$ is the rate in $\sec^{-1}$ at which state u spontaneously decays into state ℓ by emitting a photon with energy $h\nu$. The Bs are the rate coefficients in $\mathrm{cm}^3\,\sec^{-1}$ at which photons can induce transitions between the two states. $U_\nu\delta\nu$ is the local energy density of light $(\mathrm{in\,erg\,cm}^{-3})$, travelling in any direction, which is capable of inducing such transitions: that is, lying within a **bandwidth** $\delta\nu$ around the center frequency ν [1]. If in addition to steady state, the atoms or molecules and the photons are also in thermal equilibrium, we can invoke the Maxwell-Boltzmann distribution and the Planck blackbody function,

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell}\exp\left(-\frac{h\nu}{kT}\right) \qquad \text{and}$$
$$U_\nu\delta\nu = \frac{1}{c}\int_{4\pi} d\Omega\int d\nu' B_\nu\left(\nu',T\right) = \frac{8\pi h\nu^3\delta\nu}{c^3}\frac{1}{\exp\left(h\nu/kT\right)-1} \equiv \frac{C_\nu}{\exp\left(h\nu/kT\right)-1} \quad , \tag{3}$$

in the detailed-balance expression (2), to obtain

$$g_u A_{u\ell}e^{-h\nu/kT} + g_u B_{u\ell}C_\nu\frac{e^{-h\nu/kT}}{e^{h\nu/kT}-1} = g_\ell B_{\ell u}C_\nu\frac{1}{e^{h\nu/kT}-1} \quad \text{, or} \tag{4}$$

$$g_u A_{u\ell}\left(1-e^{-h\nu/kT}\right) + g_u B_{u\ell}C_\nu e^{-h\nu/kT} = g_\ell B_{\ell u}C_\nu \quad . \tag{5}$$

For this expression to work at arbitrary temperature, the terms with and without the exponential factor have to balance separately:

$$\begin{array}{ll} -g_u A_{u\ell}e^{-h\nu/kT} + g_u B_{u\ell}C_\nu e^{-h\nu/kT} = 0 & \Rightarrow \quad A_{u\ell} = B_{u\ell}C_\nu = \dfrac{8\pi h\nu^3\delta\nu}{c^3}B_{u\ell} \quad \text{and} \\ g_u A_{u\ell} = g_\ell B_{\ell u}C_\nu & \qquad g_u B_{u\ell} = g_\ell B_{\ell u} \quad . \end{array} \tag{6}$$

Because these two relations among A and the Bs are independent of temperature and density, they must apply universally, under all conditions of temperature and density, whether or not the system is in thermal equilibrium. You are already familiar with $A_{u\ell}$, the spontaneous emission rate; $B_{u\ell}$ and $B_{\ell u}$ are respectively the rate coefficients for

[1] The bandwidth $\delta\nu$ is determined by the properties of the absorbing species and the medium, as described below. In most discussions of the Einstein coefficients it is omitted, as it frequently cancels out of some subsequent equations.

stimulated emission and stimulated absorption. Collectively they are called the **Einstein A and B coefficients** [2].

With A and the Bs we can express two terms of classical radiative transfer in quantum language: our usual emission coefficient $\mathcal{J}_\nu$, which is the power per unit volume emitted isotropically at frequency ν by the medium (i.e. has units $\text{erg sec}^{-1}\ \text{cm}^{-3}$):

$$\mathcal{J}_{\nu,u\ell} = \frac{h\nu}{4\pi} A_{u\ell} n_u \quad ; \tag{7}$$

and the **absorption coefficient** κ_ν, which is the reciprocal of the mean free path of photons of frequency ν in the medium (i.e. has units cm^{-1}, unlike the form in Carroll & Ostlie which is the mass absorption coefficient):

$$\kappa_{\nu,\ell u} = \frac{h\nu}{c}\left(B_{\ell u} n_\ell - B_{u\ell} n_u\right) \quad . \tag{8}$$

As written, these coefficients represent the total emission and absorption, integrated over frequency. On a finer frequency scale, both emission and absorption are described by a profile function, which accounts for aspects of the environment which affect the range of frequencies emitted or absorbed: for example, Doppler shifts from thermal, turbulent, or systematic fluid motion.

The ratio of these two coefficients is the **source function** S_ν:

$$S_{\nu,u\ell}\delta\nu \equiv \frac{\mathcal{J}_{\nu,u\ell}}{\kappa_{\nu,u\ell}} = \frac{c}{4\pi}\frac{A_{u\ell} n_u}{B_{\ell u} n_\ell - B_{u\ell} n_u} = \frac{2h\nu^3}{c^2}\frac{1}{\frac{n_\ell g_u}{n_u g_\ell} - 1}\delta\nu \quad , \tag{9}$$

in which equation (6) was used in the last step. In thermal equilibrium (equation (3)), S_ν is the same as the Planck function $B_\nu(\nu,T)$; therefore, like the Planck function, it expresses the net power per unit area, bandwidth, and solid angle emitted by the medium. The $\delta\nu$ factor is the range of frequencies covered when the source function is integrated along with a narrow spectral-line profile centered on $\nu = \nu_{u\ell}$.

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[2] A. Einstein 1916, DeutPhysGesell 18, 318. Highly recommended reading. Charlie Townes often said that this paper was a big influence in his invention of the maser and laser.

The A and B coefficients provide a convenient way to include photon absorption and stimulated emission into the expression for nonequilibrium population ratios of molecular states under collisional excitation: the old expression

$$n_j \sum_i n_0 \gamma_{ji} + n_j \sum_{i<j} A_{ji} = \sum_i n_i n_0 \gamma_{ij} + \sum_{i>j} n_i A_{ij}$$

becomes

$$n_j \sum_i \left(n_0 \gamma_{ji} + U_\nu \delta\nu B_{ji} \right) + n_j \sum_{i<j} A_{ji} = \sum_i n_i \left(n_0 \gamma_{ij} + U_\nu \delta\nu B_{ij} \right) + \sum_{i>j} n_i A_{ij} \quad . \tag{10}$$

2. The escape probability formalism

Equation (10) can be rearranged in a more useful form by working on the energy density factor $U_\nu \delta\nu$. To wit [3,4,5]:

Neglecting free-free scattering, the intensity per unit bandwidth $I_\nu(\hat{s})$ of light at frequency ν – which has units $\mathrm{erg\ sec^{-1}\ cm^{-2}\ Hz^{-1}\ ster^{-1}}$ – travelling along unit vector $\hat{s}$, is described by the equation of radiative transfer:

$$\frac{dI_\nu(\hat{s})}{d\tau_\nu} = I_\nu(\hat{s}) - S_\nu(\hat{s}) \quad , \tag{11}$$

where the S_ν is the source function; and τ_ν is the (dimensionless) **optical depth**,

$$\tau_\nu(s) = \int_{-\infty}^{s} ds' \kappa_\nu(s') \tag{12}$$

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[3] V. Ossenkopf 1997, NewAst 2, 365, and the following two references, upon which this discussion is based.

[4] T. de Jong, S.-I. Chu, & A. Dalgarno 1975, ApJ 199, 69.

[5] N.Z. Scoville & P.M. Solomon 1974, ApJL 187, L67.

which characterizes the decrease or increase of intensity along the line of propagation $\boldsymbol{s}$. Suppose that spectral line emission and absorption is characterized by a narrow $(\Delta\nu \ll \nu)$ profile [6], so that

$$S_\nu(\hat{s}) = S_0\varphi(\nu',\hat{s}) \quad , \quad \int_{-\infty}^{\infty} d\nu'\varphi(\nu',\hat{s}) = \delta\nu \quad . \tag{13}$$

The solution to equation (11) is

$$I_\nu(\boldsymbol{s}) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} d\tau'_\nu S_\nu(\boldsymbol{s}')e^{\tau'_\nu-\tau_\nu} \quad . \tag{14}$$

where now the terms depend on the entire path of light propagation, rather than just the local direction as in equations (11)-(13).

This would be the beginning of a hard problem, as the source function is in general a function of τ'_ν through $\boldsymbol{s}'$ and $\kappa_\nu(\boldsymbol{s}')$ [7]. Let's assume, however, that it is independent of τ'_ν; then it comes out of the integral, we can drop reference to dependence upon $\boldsymbol{s}'$, and we get

$$I_\nu(\boldsymbol{s}) = I_\nu(0)e^{-\tau_\nu} + S_\nu(0)\left(1-e^{-\tau_\nu}\right) \quad . \tag{15}$$

The bold or naïve step of assuming that S_ν can come out of the integral is called the **Sobolev approximation** [8]. In these terms we can write the energy density $U_\nu\delta\nu$ as

[6] We need not specify the profile, but if a concrete example helps, use a Gaussian, $\varphi(\nu',\hat{s}) = \exp\left(-[\nu'-\nu]/\delta\nu^2\right)/\sqrt{\pi}$, with $\delta\nu \ll$ the line-center frequency $\nu = \nu_{u\ell}$. As written, its integral over frequency is $\delta\nu$.

[7] When the valid approximations can't simplify this expression significantly, we normally construct a model for the absorbing/emitting medium; return to equation (17); integrate it numerically, at great computational cost; and iterate by changing the model until constraints such as observations are satisfied.

[8] V.V. Sobolev 1963, *A treatise on radiative transfer* (Princeton: Van Nostrand). Some refer to this step as the escape-probability approximation.

$$U_\nu \delta\nu = \int_{4\pi} d\Omega \left(\frac{1}{c} \int_{-\infty}^{\infty} d\nu' I_\nu \varphi(\nu') \right)$$

$$= \frac{I_\nu(0)}{c} \int_{4\pi} d\Omega \int_{-\infty}^{\infty} d\nu' \varphi(\nu') e^{-\tau_{\nu'}} + \frac{S_\nu(0)}{c} \int_{4\pi} d\Omega \int_{-\infty}^{\infty} d\nu' \varphi(\nu') \left(1 - e^{-\tau_{\nu'}}\right) \quad ,$$

or

$$U_\nu = \frac{4\pi I_\nu(0)}{c} \beta + \frac{4\pi S_\nu(0)}{c} (1-\beta) \quad , \tag{16}$$

where

$$\beta \equiv \int_{4\pi} \frac{d\Omega}{4\pi} \int_{-\infty}^{\infty} \frac{d\nu'}{\delta\nu} \varphi(\nu') e^{-\tau_{\nu'}} \tag{17}$$

is called the **escape probability**. As can be seen from its form, it gives the probability that a photon emitted within the medium makes to the surface and escapes, maybe to the observer: if $\beta = 1$, then $U_\nu = 4\pi I_\nu(0)/c$, as if the medium is transparent; while if $\beta = 0$, then $U_\nu = 4\pi S_\nu(0)/c$, which in thermal equilibrium reduces to the energy density per unit bandwidth in blackbody radiation, as in equation (3), and as it should.

The escape probability is much easier to calculate than the integral in equation (14).

3. The large velocity gradient approximation

A surprisingly large variety of problems yield to the Sobolev approximation [9]. One common situation where it applies is a medium with a monotonic **large velocity gradient** (**LVG***)*. This is what Sobolev had in mind when he invented the escape-probability formalism, in expanding, spherical atmospheres of giant stars. It also describes cooling behind interstellar shocks, as there is a large velocity change between the jump and the end state of post-shock gas cooling.

Consider a horizontal plane-parallel layer, thickness *z*, with a large vertical flow-velocity gradient, and calculate the escape probability for light emitted at an angle θ from normal (Figure 1). By large, we mean in comparison to the thermal speed, $v_t = \sqrt{3kT/m}$, where m is the molecular mass. Along a path s at angle θ from the vertical, the flow velocity is less than the vertical by the factor $\cos\theta$. An inclined path through the layer is longer than the vertical path to the same level by a factor of $1/\cos\theta$. So the velocity gradient along this path is smaller than that in the vertical direction:

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[9] See D.A. Neufeld & G.J. Melnick 1991, ApJ 368, 215, for uses of the escape probability formalism beyond the LVG approximation.

$$\frac{dv_s}{ds} = \cos^2\theta \frac{dv}{dz} \quad . \tag{18}$$

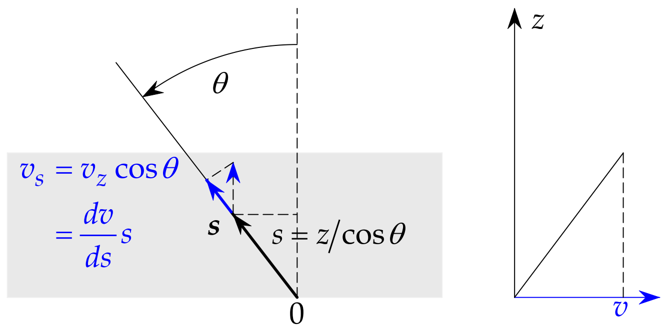

Figure 1: geometry of spectral-line emission and absorption in a plane-parallel layer (left) with a large velocity gradient (depicted at right).

At a point a distance s further down the path, the medium's absorption profile is Doppler shifted redward by a frequency

$$\Delta\nu = \nu\frac{\Delta v_s}{c} = \nu\cos^2\theta\frac{1}{c}\frac{dv}{dz}s \quad . \tag{19}$$

Instead of facing absorption centered at frequency ν, light will be absorbed at frequencies centered on $\nu - \Delta\nu$. Suppose the frequency dependence of line absorption is

$$\kappa_{\nu'} = \kappa_{\nu',\ell u}\varphi\left(\nu' - \nu\right) \quad . \tag{20}$$

The optical depth of the medium between the starting point and the surface becomes

$$\tau_\nu = \int_0^{z/\cos\theta} ds'\kappa_{\nu',\,\ell u}\varphi\left(\nu' - \nu + \nu\cos^2\theta\frac{1}{c}\frac{dv}{dz}s'\right) \quad . \tag{21}$$

If $\Delta\nu$ is larger than $\nu' - \nu$, then the value of φ is very small, so a large dv/dz reduces the optical depth toward the observer from the starting point; **only the region close to the starting point contributes significantly to the optical depth**. This simplifies the integrals –the upper bounds can be extended to infinity – and also makes the Sobolev approximation a good one: the source function and absorption coefficient can be taken to vary negligibly within this region, and can therefore come out of the integrals in equations (14) and (21).

To evaluate the optical depth in equation (21), substitute variables as follows:

$$\begin{aligned}
\nu_1 &= -\nu' + \nu \\
\nu_1' &= -\nu_1 + \nu\cos^2\theta \frac{1}{c}\frac{dv}{dz}s' \\
d\nu_1' &= \nu\cos^2\theta \frac{1}{c}\frac{dv}{dz}ds' \\
\nu_1' &= -\nu_1 \rightarrow \infty \text{ as } s' = 0 \rightarrow \infty
\end{aligned} \tag{22}$$

to get
$$\tau_\nu\left(\nu_1\right) = \frac{c\kappa_{\nu,\ell u}}{\nu\, dv/dz}\frac{1}{\cos^2\theta}\int_{-\nu_1}^{\infty} d\nu_1'\varphi\left(\nu_1'\right) \equiv t\frac{1}{\cos^2\theta}\int_{-\nu_1}^{\infty} d\nu_1'\varphi\left(\nu_1'\right) \quad . \tag{23}$$

This is ready to put in the expression for escape probability, equation (17). Use again the first substitution from equation (22):

$$\beta_{u\ell} = \int_{4\pi}\frac{d\Omega}{4\pi}\int_{-\infty}^{\infty}\frac{d\nu'}{\delta\nu}\varphi\left(\nu'-\nu\right)e^{-\tau_{\nu'}\left(\nu'-\nu\right)} = \int_{4\pi}\frac{d\Omega}{4\pi}\int_{\infty}^{-\infty}\frac{d\nu_1}{\delta\nu}\varphi\left(\nu_1\right)e^{-\tau_\nu\left(\nu_1\right)} \quad . \tag{24}$$

Recall the way the line profile is normalized, equation (13), along with the fundamental theorem of calculus, and substitute

$$\begin{aligned}
x &= \int_{-\nu_1}^{\infty} d\nu_1'\varphi\left(\nu_1'\right) \\
dx &= -\varphi\left(\nu_1\right)d\nu_1 \\
x &= 0 \rightarrow \delta\nu \text{ as } x = \infty \rightarrow -\infty
\end{aligned} \tag{25}$$

to produce

$$\beta_{u\ell} = \frac{1}{4\pi\delta\nu}\int_0^{2\pi} d\phi\int_0^{\pi} d\theta\sin\theta\int_0^{\delta\nu} dx\exp\left(-\frac{tx}{\cos^2\theta}\right) \quad . \tag{26}$$

Simplify by doing the (trivial) azimuthal integral, and substituting

$$\begin{aligned}
&\mu = \cos\theta, \quad d\mu = -\sin\theta d\theta \quad , \\
&\mu = 1 \rightarrow -1 \text{ as } \theta = 0 \rightarrow \pi \quad :
\end{aligned} \tag{27}$$

$$\begin{aligned}
\beta_{u\ell} &= \frac{1}{2\delta\nu}\int_{-1}^{1} d\mu\int_0^{\delta\nu} dx\exp\left(-\frac{tx}{\mu^2}\right) \\
&= \frac{1}{2}\int_{-1}^{1} d\mu\left[-\frac{\mu^2}{t\delta\nu}\exp\left(-\frac{tx}{\mu^2}\right)\right]_0^{\delta\nu} = \frac{1}{2}\int_{-1}^{1} d\mu\frac{\mu^2}{t\delta\nu}\left(1-e^{-t\delta\nu/\mu^2}\right) \quad .
\end{aligned} \tag{28}$$

Now define

$$\tau_{\ell u} \equiv t\delta\nu = \frac{c\kappa_{\nu,\ell u}\delta\nu}{\nu\, dv/dz} = \frac{c\delta\nu}{\nu\, dv/dz}\frac{h\nu}{c}\frac{c^3 A_{u\ell}}{8\pi h\nu^3\delta\nu}\left(\frac{g_u n_\ell}{g_\ell} - n_u\right)$$
$$= \frac{c^3 A_{u\ell} n}{8\pi\nu^3\, dv/dz}\left(\frac{g_u f_\ell}{g_\ell} - f_u\right) \quad , \tag{29}$$

where n is the number density of the absorbing species and the *f*s are the population fractions in the states indicated, and obtain [10]

$$\beta_{u\ell} = \frac{1}{2}\int_{-1}^{1} d\mu \frac{1-\exp\left(-\tau_{\ell u}/\mu^2\right)}{\left(\tau_{\ell u}/\mu^2\right)} \quad . \tag{30}$$

There are two choices forward from here. The first and most common [4,5] is to assume both factors μ^2 in the integrand to be the values of $\mu^2 = \cos^2\theta$ averaged over all solid angles, as if applying this averaging process in equation (18). In this case, $\left\langle \mu^2 \right\rangle = 1/3$, and

$$\beta_{u\ell} = \frac{1-\exp\left(-3\tau_{\ell u}\right)}{3\tau_{\ell u}} \quad . \tag{31}$$

This satisfies the limits on $\beta_{u\ell}$ at the extremes of $\tau_{\ell u}$:

$$\lim_{\tau_{\ell u}\to 0} \beta_{u\ell} = 1, \quad \lim_{\tau_{\ell u}\to\infty} \beta_{u\ell} = 0,$$

as expected. The other choice is to work the integrals out; that is, average over direction now, not earlier in the calculation, which is somewhat more defensible. The first integral includes the average of μ^2 over solid angle, demonstrating that it is $1/3$; I looked the second one up in Wolfram Alpha:

[10] At this point, the factors of $\delta\nu$ have cancelled out. This is an example of why many leave them out of the whole derivation for simplicity, and don't worry about the dimensions before the final result.

$$\beta_{u\ell} = \frac{1}{3\tau_{\ell u}} - \left[\frac{\mu^3 e^{-\tau_{\ell u}/\mu^2}}{6\tau_{\ell u}} - \frac{\mu e^{-\tau_{\ell u}/\mu^2}}{3} - \frac{\sqrt{\pi\tau_{\ell u}}}{3} \operatorname{erf}\left(\sqrt{\frac{\tau_{\ell u}}{\mu^2}} \right) \right]_{-1}^{1}$$
$$= \frac{1}{3\tau_{\ell u}} - \left[\frac{e^{-\tau_{\ell u}}}{3\tau_{\ell u}} - \frac{2e^{-\tau_{\ell u}}}{3} \right] = \frac{1-(1-2\tau_{\ell u})e^{-\tau_{\ell u}}}{3\tau_{\ell u}} \quad . \tag{32}$$

Again we examine the limits, to find

$$\lim_{\tau_{\ell u}\to 0} \beta_{u\ell} = 1, \quad \lim_{\tau_{\ell u}\to\infty} \beta_{u\ell} = 0,$$

also as expected. So it matters at which point in the calculation one integrates over the angles. But not by very much; the two functions differ by about 10% at most and usually by much less than 1% (Figure 5). One is no easier to calculate than the other. We will use equation (31), for ease of comparison to earlier work, but note that equation (32) is more nearly correct.

That the escape probability is "contained" within $\cos^2\theta = 1/3$ $(\theta = 33°)$ has observational consequences: it means that opaque spectral lines from a plane-parallel LVG layer are dimmer when viewing the layer obliquely than when viewing it face-on. This is a well known feature of the **Eddington approximation**, which many equate with the statement $\left\langle \cos^2\theta \right\rangle = 1/3$; it is the explanation for the Sun's limb darkening, for example.

The escape probability can be applied to any photon emitted in the prescribed medium, and to any photon incident from elsewhere, as in equation (14): **all the $A_{u\ell}$ factors in equation (10) can simply be replaced by $\beta_{u\ell} A_{u\ell}$**. Neglect, to good approximation, background incident light (i.e. take $I_\nu(0) = 0$), such as starlight and the cosmic background; this eliminates the remaining B-coefficient terms. This leaves a familiar-looking system of equations to solve for the energy-level densities n_j :

$$n_j \sum_i n_0 \gamma_{ji} + n_j \sum_{i<j} \beta_{ji} A_{ji} = \sum_i n_i n_0 \gamma_{ij} + \sum_{i>j} n_i \beta_{ij} A_{ij} \quad , \tag{33}$$

where
$$\beta_{ji} = \frac{1-e^{-3\tau_{ij}}}{3\tau_{ij}} \tag{34}$$

and
$$\tau_{ij} = \frac{c\kappa_{\nu,ij}}{\nu_{ji}\left(dv/dz\right)} = \frac{c^3 A_{ji} n}{8\pi\nu_{ji}^3 \, dv/dz} \left(\frac{g_j f_i}{g_i} - f_j \right) \quad . \tag{35}$$

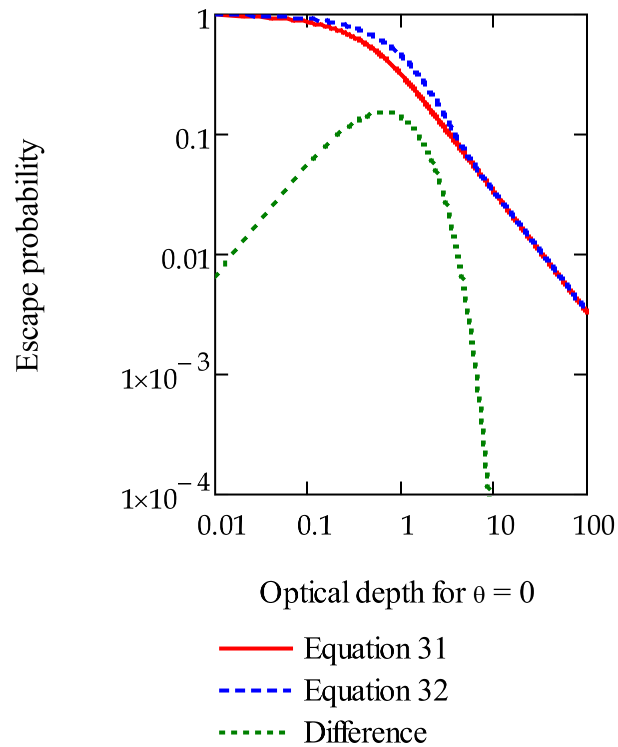

Figure 2: comparison of the two slightly different forms of $\beta_{u\ell}$ derived in section 3.

