Sobolev Escape Probability Bound-bound Rates

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1 Overview

Our goal is to obtain an expression for the rate of transitions (transitions s^{-1} cm^{-3}) that occur due to a bound-bound transition in the Sobolev approximation. These rates are needed for things like solving the statistical equilibrium equations (to obtain NLTE level populations) of for Macro Atom transition probabilities.

The net rate of transitions from lower atomic level l to upper level u due to a bound-bound transition between the levels can be written:

$$R_{l \rightarrow u} = (n_l B_{lu} - n_u B_{ul}) \bar{J}_{lu} - n_u A_{ul} \tag{1}$$

where B and A are the usual Einstein coefficients, ns are the level populations (cm^{-3}) and

$$\bar{J}_{lu} = \int_{-\infty}^{\infty} J(\nu) \phi_{lu}(\nu) \, \mathrm{d}\nu \tag{2}$$

is the "mean intensity in the line": specifically, it is the mean intensity (integral of specific intensity over solid angle)

$$J(\nu) = \frac{1}{4\pi} \int I(\nu, \underline{\mathrm{n}}) \, \mathrm{d}\Omega \tag{3}$$

integrated over frequency weighted by the line *absorption* profile $\phi_{lu}(\nu)$. Recall that $\phi_{lu}(\nu)$ will be a function that is sharply peaked around the line frequency ν_{ul} and the Sobolev approximation can be (loosely) stated as the case that $\phi_{lu}(\nu)$ tends towards the delta function.

Conceptually, we would normally consider the first term in equation 1 (the B-terms) as being "absorption" (where stimulated emission is treated as negative absorption) and the second term (the A-term, which is negative) as being "emission". We note that for statistical equilibrium and/or macro atom probabilities this identification does not matter: all we require is that the net rate of transitions is correctly represented (and, for macro atoms, any term we identify with a transition probability must be positive, of course).

So far, nothing has been specific to the Sobolev limit. In the following I'll introduce that approximation. Throughout we will now consider ν to be a comoving frequency and, except where specifically noted, consider that all quantities should be evaluated at the Sobolev point (in the frame co-moving with the Sobolev point). Note that the populations (ns) and the intensities (I, J, $\bar{J}$) all depend on position. However, I will not include this in the notation: it is to be understood that all these quantities implicitly depend on position and we consider the following analysis to be at a specific point.

2 Sobolev assumptions

In the presence of steep velocity gradients, we assume that interaction between a ray ($I(\nu, \underline{\mathrm{n}})$) and the line is restricted to a (vanishingly) small region (Sobolev region) in which the co-moving frame frequency of photons in the ray is sufficiently close to ν_{ul} that $\phi_{ul}(\nu)$ is non-negligible. As the ray passes through the Sobolev region, the pathlength traversed is related to the co-moving frame frequency interval swept out in the usual Sobolev way:

$$\mathrm{d}s = \left|\frac{\mathrm{d}s}{\mathrm{d}\nu}\right| \mathrm{d}\nu = g(\underline{\mathrm{n}})\mathrm{d}\nu \ \ . \tag{4}$$

Here, we introduce $g(\underline{\mathrm{n}})$ as notation for the inverse gradient of co-moving frame frequency with pathlength, explicitly noting that it depends on the direction of propagation of the ray ($\underline{\mathrm{n}}$), which will be a key fact in our story[1].

We also introduce the total Sobolev optical depth encountered by this same ray in traversing the entire Sobolev region:

$$\tau_s(\underline{\mathrm{n}}) = \frac{h\nu_{ul}}{4\pi}(n_l B_{lu} - n_u B_{ul})g(\underline{\mathrm{n}}) = \kappa_{lu} g(\underline{\mathrm{n}}) \ \ . \tag{5}$$

where we introduce

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

We note that (i) τ_s also depends on $\underline{\mathrm{n}}$ and (ii) this dependence is entirely due to g (no other quantities in this expression depend on the direction of the ray).

3 Calculation of $\bar{J}$

We now with to evaluate $\bar{J}_{lu}$ in the Sobolev limit. Combining equations 2 and 3 and reversing the order of the integration gives us:

$$\bar{J}_{lu} = \frac{1}{4\pi}\int \left(\int_{-\infty}^{\infty} I(\nu, \underline{\mathrm{n}})\phi_{lu}(\nu)\ \mathrm{d}\nu\right) \mathrm{d}\Omega \tag{7}$$

In the end we will be interpreting this as an angular integral over rays that come into Sobolev resonance with the line at our point of interest. So we will first tackle the inner integral, which is where magical things happen. Consider:

$$\int_{-\infty}^{\infty} I(\nu, \underline{\mathrm{n}})\phi_{lu}(\nu)\ \mathrm{d}\nu \ \ . \tag{8}$$

To evaluate this, we need to know $I(\nu, \underline{\mathrm{n}})$ *within* the Sobolev region. I.e. we need to know how $I(\nu, \underline{\mathrm{n}})$ changes across the profile function. To do this, we use the radiative transfer equation, expressed in terms of path length along the ray (we are working now in the frame that is formally co-moving with the Sobolev point):

$$\frac{\mathrm{d}I(\nu, \underline{\mathrm{n}})}{\mathrm{d}s} = -\kappa(\nu)I(\nu, \underline{\mathrm{n}}) + \epsilon(\nu) \tag{9}$$

where $\kappa(\nu)$ is the absorption co-efficient and $\epsilon(\nu)$ the emissivity. We now made the *isolated line* approximation: assume that both opacity and emissivity within the Sobolev region are dominated by the bound-bound transition under consideration. Thus:

[1]Note that I have used the modulus of the gradient here. One can instead introduce a negative sign to the definition of path length, but I want to remain general: make no fixed statement about whether the ray will blueshift or redshift through the Sobolev region. The assumption is only that the velocity gradient is assumed to be a *constant* for any particular ray as it passes through the Sobolev region. In principle, however, it can have either positive or negative sign.

$$\kappa(\nu) = \frac{h\nu_{ul}}{4\pi}(n_l B_{lu} - n_u B_{ul})\phi_{lu}(\nu) = \kappa_{lu}\phi_{lu}(\nu) \tag{10}$$

and

$$\epsilon(\nu) = \frac{h\nu_{ul}}{4\pi} n_u A_{ul}\eta_{ul}(\nu) = \epsilon_{ul}\eta_{ul}(\nu) \tag{11}$$

where we now introduce

$$\epsilon_{ul} = \frac{h\nu_{ul}}{4\pi} n_u A_{ul} \tag{12}$$

and an emission profile $\eta_{ul}(\nu)$. I have made an implicit assumption here, namely that the stimulated emission profile (relevant to equation 10) is the same as the absorption profile, $\phi_{lu}(\nu)$. We will immediately also make the equivalent (and more important) assumption (CRD) that the *spontaneous* emission profile is the same as the absorption profile:

$$\eta_{ul}(\nu) = \phi_{lu}(\nu) \quad . \tag{13}$$

Using equations 10 and 11 in equation 9 gives:

$$\mathrm{d}I(\nu, \underline{\mathrm{n}}) = -\kappa_{lu}\phi_{lu}(\nu) I(\nu, \underline{\mathrm{n}})\ \mathrm{d}s + \epsilon_{ul}\eta_{ul}(\nu)\ \mathrm{d}s \tag{14}$$

We can introduce an optical depth variable to describe the ray traversing the Sobolev region:

$$\mathrm{d}\tau = \kappa_{lu}\phi_{lu}(\nu)\ \mathrm{d}s \tag{15}$$

and so obtain:

$$\mathrm{d}I(\nu, \underline{\mathrm{n}}) = -I(\nu, \underline{\mathrm{n}})\ \mathrm{d}\tau + \frac{\epsilon_{ul}}{\kappa_{lu}}\ \mathrm{d}\tau \tag{16}$$

where we have made use of equation 13 to cancel $\eta_{ul}(\nu)$ out from the last term. Since within the (small) Sobolev region the line source function

$$S_{lu} = \frac{\epsilon_{ul}}{\kappa_{lu}} = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} \tag{17}$$

can be taken as a constant, this is just the simplest form of the RT equation:

$$\frac{\mathrm{d}I(\nu, \underline{\mathrm{n}})}{\mathrm{d}\tau} = -I(\nu, \underline{\mathrm{n}}) + S_{lu} \tag{18}$$

for which the formal solution is well known:

$$I(\nu, \underline{\mathrm{n}}) = I_0(\underline{\mathrm{n}})e^{(-\tau)} + S_{lu}(1 - e^{(-\tau)}) \tag{19}$$

where $I_0(\underline{\mathrm{n}})$ is the intensity of the ray as it starts to encounter the opacity (in our case, as it enters the Sobolev region). We may now return to equation 8 and use this expression for the specific intensity inside the Sobolev region:

$$\int_{-\infty}^{\infty} I(\nu, \underline{\mathrm{n}})\phi_{lu}(\nu)\ \mathrm{d}\nu = \int_{-\infty}^{\infty} (I_0(\underline{\mathrm{n}})e^{(-\tau)} + S_{lu}(1 - e^{(-\tau)}))\phi_{lu}(\nu)\ \mathrm{d}\nu \quad . \tag{20}$$

We now realise that, in the Sobolev limit, the integral over frequency here can be cast as an integral over optical depth since as a ray traverses the Sobolev region it sweeps out frequency space and optical depth space (and indeed pathlength, ds) simultaneously. Specifically, if we combine equation 4 with 15 and then make use of equation 5 we obtain[2]

$$\mathrm{d}\tau = \kappa_{lu}\phi_{lu}(\nu)g(\underline{\mathrm{n}})\ \mathrm{d}\nu = \tau_s(\underline{\mathrm{n}})\phi_{lu}(\nu)\mathrm{d}\nu \quad . \tag{21}$$

Using this in equation 20 gives:

$$\int_{-\infty}^{\infty} I(\nu,\underline{\mathrm{n}})\phi_{lu}(\nu)\ \mathrm{d}\nu = \int_{0}^{\tau_s(\underline{\mathrm{n}})} (I_0(\underline{\mathrm{n}})e^{(-\tau)} + S_{lu}(1-e^{(-\tau)}))\frac{1}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\tau \quad . \tag{22}$$

Given that $I_0(\underline{\mathrm{n}})$ is a constant and assuming that the Sobolev region is sufficiently small that we can take S_{lu}, κ_{lu} and $g(\underline{\mathrm{n}})$ as constants, this integral is do-able:

$$\int_{-\infty}^{\infty} I(\nu,\underline{\mathrm{n}})\phi_{lu}(\nu)\ \mathrm{d}\nu = I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})} + S_{lu}\frac{\tau_s(\underline{\mathrm{n}}) + e^{(-\tau_s(\underline{\mathrm{n}}))}-1}{\tau_s(\underline{\mathrm{n}})} \tag{23}$$

Now having a concrete expression for this integral, we can return to equation 7 and substitute for the inner integral:

$$\bar{J}_{lu} = \frac{1}{4\pi}\int \left(I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})} + S_{lu}\frac{\tau_s(\underline{\mathrm{n}}) + e^{(-\tau_s(\underline{\mathrm{n}}))}-1}{\tau_s(\underline{\mathrm{n}})} \right) \mathrm{d}\Omega \tag{24}$$

Since S_{lu} is a constant (no angular dependence) it is natural to separate out the terms:

$$\bar{J}_{lu} = \frac{1}{4\pi}\int I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \ \ + \frac{S_{lu}}{4\pi}\int \frac{\tau_s(\underline{\mathrm{n}}) + e^{(-\tau_s(\underline{\mathrm{n}}))}-1}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \tag{25}$$

or

$$\bar{J}_{lu} = \frac{1}{4\pi}\int I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \ \ + S_{lu} + \frac{S_{lu}}{4\pi}\int \frac{e^{(-\tau_s(\underline{\mathrm{n}}))}-1}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \tag{26}$$

We can immediately see that this is useful: we now have (i) a first term that depends on an angle integration of the intensity distribution of rays coming into Sobolev resonance (the distribution of $I_0(\underline{\mathrm{n}})$) with a weighting factor; and (ii) a second term this is just the source function and (iii) a third term that is independent of the angular distribution of incoming rays but depends on the angular distribution of τ_s.

4 The Point

Why did we do the above? ...to calculated the net radiative rate given by equation 1:

$$R_{l\rightarrow u} = (n_l B_{lu} - n_u B_{ul})\bar{J}_{lu} - n_u A_{ul} \quad . \tag{27}$$

Using equation 26 in this expression we have at last:

$$R_{l\rightarrow u} = (n_l B_{lu} - n_u B_{ul})\left(\frac{1}{4\pi}\int I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \ \ + S_{lu} - \frac{S_{lu}}{4\pi}\int \frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \right) - n_u A_{ul} \quad . \tag{28}$$

Making use of equation 17, we see that

$$(n_l B_{lu} - n_u B_{ul})S_{lu} = n_u A_{ul} \tag{29}$$

[2]Note that $\tau_s(\underline{\mathrm{n}})$ is simply obtained by integrating this equation over all ν, assuming that $\phi_{lu}(\nu)$ is sharply peaked.

and so the second term that emerged in our expression for $\bar{J}_{lu}$ exactly cancels the original spontaneous emission term. Thus we are left with two terms in the net rate:

$$R_{l\to u} = (n_l B_{lu} - n_u B_{ul})\frac{1}{4\pi}\int I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega \quad - n_u A_{ul}\frac{1}{4\pi}\int \frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega\ \ . \tag{30}$$

and this is our final expression: it gives the net transition rate in the Sobolev approximation as a sum of two terms. Assuming that stimulated emission can be treated as negative absorption, we interpret the first term as an *effective absorption* rate and the second as an *effective emission* rate.

4.1 Emission term

Specifically, we identify the rate of emission (transitions s^{-1} cm^{-3}) with[3]

$$n_u A_{ul}\frac{1}{4\pi}\int \frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega = n_u A_{ul}\beta_{\mathrm{esc}} \tag{31}$$

where, if we introduce

$$p_{\mathrm{esc}}(\underline{\mathrm{n}}) = \frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})} \tag{32}$$

we can now identify

$$\beta_{\mathrm{esc}} = \frac{1}{4\pi}\int p_{\mathrm{esc}}(\underline{\mathrm{n}})\ \mathrm{d}\Omega \tag{33}$$

as the *angle-averaged Sobolev escape probability*.

This discussion of the effective emission term does not depend on any isotropy assumption of the radiation field. We note that in the particular case where $\tau_s(\underline{\mathrm{n}}) = \tau_s$ is angle-independent, then the integral will be trivial and

$$\beta_{\mathrm{esc}} = \frac{1-e^{(-\tau_s)}}{\tau_s}\ \ . \tag{34}$$

4.2 Absorption term

The term describing the effective absorption rate is identified as

$$(n_l B_{lu} - n_u B_{ul})\frac{1}{4\pi}\int I_0(\underline{\mathrm{n}})\frac{1-e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})}\ \mathrm{d}\Omega = (n_l B_{lu} - n_u B_{ul})\frac{1}{4\pi}\int I_0(\underline{\mathrm{n}})p_{\mathrm{esc}}(\underline{\mathrm{n}})\ \mathrm{d}\Omega \tag{35}$$

Here we see that the situation is complicated since both the distribution of intensity of the rays coming into resonance at the Sobolev point ($I_0(\underline{\mathrm{n}})$) *and* $p_{\mathrm{esc}}(\underline{\mathrm{n}})$ are angle dependent. We cannot therefore easily break up the integral unless either $p_{\mathrm{esc}}(\underline{\mathrm{n}})$ is isotropic (as in e.g. a homologous flow [i.e. supernovae]) *or* the incoming radiation field is isotropic.

4.2.1 Homologous flow case

In e.g. supernovae, if the velocity field is well-approximated by homologous expansion then (i) $\tau_s(\underline{\mathrm{n}}) = \tau_s$ is angle independent and (ii) the co-moving frequency of all rays is continuously red-shifting. In that case, the effective absorption term is:

[3] Note the sign change here: this is because we interpret the total rate as absorption *minus* emission.

$$(n_l B_{lu} - n_u B_{ul}) \frac{1 - e^{(-\tau_s)}}{\tau_s} \frac{1}{4\pi} \int I_0(\underline{\mathrm{n}}) \; \mathrm{d}\Omega \tag{36}$$

and we can identify the integral:

$$J_b = \frac{1}{4\pi} \int I_0(\underline{\mathrm{n}}) \; \mathrm{d}\Omega \tag{37}$$

as the *mean intensity at the far blue wing of the line*: it is the angle-integral over the specific intensity of rays that are Doppler shifting into Sobolev resonance, which is the "blue" wing since all rays are Doppler shifting towards the red. This is the form used in the supernova work, specifically in Lucy's supernova papers: i.e.

$$\text{absorption rate} = (n_l B_{lu} - n_u B_{ul}) \frac{1 - e^{(-\tau_s)}}{\tau_s} J_b \tag{38}$$

In Lucy (2003), a specific form is given for a Monte Carlo estimator to obtain J_b by recording the properties of Monte Carlo packets as they come into Sobolev resonance.

This is also the approach/form used in TARDIS.

4.2.2 Stellar winds

In a simple (outwards acceleration) spherical stellar wind, the identification of I_0 with the blue wing of the line is still valid, but $\tau_s(\underline{\mathrm{n}})$ (and therefore $p_{\mathrm{esc}}(\underline{\mathrm{n}})$) retain angle dependence. In this case we cannot significantly simplify

$$\text{absorption rate} = (n_l B_{lu} - n_u B_{ul}) \frac{1}{4\pi} \int I_0(\underline{\mathrm{n}}) p_{\mathrm{esc}}(\underline{\mathrm{n}}) \; \mathrm{d}\Omega \ . \tag{39}$$

In Sim (2004) I approached this by using an estimator similar to Lucy (2003) but retaining the factor

$$p_{\mathrm{esc}}(\underline{\mathrm{n}}) = \frac{1 - e^{(-\tau_s(\underline{\mathrm{n}}))}}{\tau_s(\underline{\mathrm{n}})} \tag{40}$$

inside the estimator. A physical interpretation of the quantity given by this estimator is harder to give (compared to Lucy's *mean intensity at the blue wing*), but I believe that the generalisation is appropriate and doesn't involve making any additional symmetry assumption about τ_s or I_0.

4.2.3 Python implementation

The Python (Long & Knigge 2002) implementation of estimators (made for use in Sim et al. 2005) should be very similar to the stellar wind case described above. Again

$$\text{absorption rate} = (n_l B_{lu} - n_u B_{ul}) \frac{1}{4\pi} \int I_0(\underline{\mathrm{n}}) p_{\mathrm{esc}}(\underline{\mathrm{n}}) \; \mathrm{d}\Omega \tag{41}$$

and we should not (do not?!) make any symmetry assumption and so cannot break the integral. Nevertheless, we use the same sort of estimator as used in the Sim et al. (2004) stellar winds work. The conceptual difference now is that even the identification with the *blue wing* of the line is not valid: in Python, trajectories can have co-moving frame frequencies that either red-shift *or* blue-shift and so we have to regard $I_0(\underline{\mathrm{n}})$ merely as the specific intensity distribution of all rays that Dopper shift into Sobolev resonance, regardless of whether they come in from the red or the blue. However, by using the modulus of the gradient in the formalism here, this makes no difference to the form of the estimator or the validity of the approximations.

In Python we also shift the stimulated emission term back to be a positive emission term (rather than a negative absorption term). That has no practical consequence, however, provided that stimulated emission is weaker than stimulated absorption. So long as the CRD assumption is held, the $\bar{J}$ quantity that is relevant for stimulated emission is exactly the same one as for stimulated absorption. (And if the CRD assumption is not valid, then all hell would break loose anyway.)

4.3 Approximations made

Having gone through all that, here is the list of approximations that I think we've made:

- Isolated line approximation
- CRD (absorption profile, stimulated emission profile and spontaneous emission profile all assumed equal)
- Sobolev limit
- Neglect all Doppler factors/frame-transformations *except* the one that is key to the Sobolev approximation

It seems to me that none of these assumptions is serious, or what the referee is likely to be getting at. The last one is the one I understand least well, but I don't think it has anything to do with isotropy.

Note that, for use in Python, we are effectively assuming that the velocity gradient along a ray is constant throughout the Sobolev region. And we should also note that the Sobolev approximation will be violated for some rays (since, in any of our disk wind cases, there are some rays along which the velocity gradient is not always large – but I see no particular reason to be any more concerned about that here than in any other aspects of Python's treatment of line processes).