

Calculating Spectra of Supernovae, Kilonovae and other Expanding Transients: A worksheet

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This worksheet guides the reader through some basic calculations helpful for understanding basic spectrum formation in supernovae. It also provides recipes for writing relatively simple codes to calculate synthetic model line profiles and spectra. The methods can be helpful for analyzing observed supernova spectra and making approximate predictions of the spectral signatures of explosion models (even aspherical ones!).

This [git hub repo](#) provides lists (kurucz_lines_cd23.dat) of atomic line transitions that can be used via the equations below to determine which lines are important in a spectrum. The repo also includes a useful python script, *snlines.py* that aids in identifying lines in observed supernova spectra and estimating expansion velocities.

WE WILL FOLLOW THE “ELEMENTARY SUPERNOVA MODEL”, which is similar to that used in the well known *Synow* code. We make several simplifying assumptions:

Assumption 1: The continuum is produced by a sharp¹ black-body photosphere of temperature T_{ph} , which emits a constant intensity $I_p = B_\lambda(T_{\text{ph}})$ in all directions. The photospheric temperature could be estimated from Stefan’s law $L = 4\pi R_{\text{ph}}^2 \sigma_{\text{sb}} T_p^4$, with σ_{sb} the Stefan-Boltzmann constant. For the purposes of this exercise, we take L and R_{ph} as given.²

Assumption 2: We ignore time-dependence and only calculate a “snapshot” of the spectrum at some time t after the explosion. This is often called the *stationarity* assumption³. Since the ejecta is optically thin in the continuum above the photosphere, the travel time for a photon to escape the ejecta (at an outer radius $r = r_{\text{max}}$) is $t_{lc} = r_{\text{max}}/c = v_{\text{max}}t/c$ which is short compared to the expansion time t_{exp} as long as $v_{\text{max}} \ll c$.

Assumption 3: The ejecta is in homologous expansion, where the velocity, v , at any radius, r is given by $v(r) = r/t$. (Actually, the formalism here can be generalized to other velocity laws, although the mathematics becomes somewhat more complicated.)

Expansion of the ejecta has a dramatic effect on line radiation transport. Imagine a photon emitted from the photosphere. As the photon propagates through the ejecta, it moves into regions of differing velocities. Hence, its wavelength *with respect to the co-moving frame*⁴ is constantly Doppler shifting. If

¹ We define the photosphere as the radius at which the continuum optical depth $\tau = 1$. In reality, of course, the photosphere is not a sharp surface, rather there is a gradual transition from optically thick to optically thin, and the location of $\tau \approx 1$ can depend on wavelength.

² See my other set of notes *Calculating Analytic Light Curves of Supernovae, Kilonovae, and Other Transients: A worksheet* for methods for calculating L and R_{ph} . Alternatively, these values could be adjusted to fit an observed event.

³ In contrast to the “static” approximation, the stationarity approximation takes into account the fact that the ejecta is moving – this is crucial for considering the Doppler shift effects which set the line profiles. Rather, stationary simply assumes that the amount the ejecta moves or changes is negligible on the timescale of interest.

⁴ By co-moving frame wavelength we mean the wavelength of the photon measured in a frame moving along with ejecta at that particular point in space.

a photon initially has a wavelength λ_{cmf} in the local co-moving frame, then after moving some distance Δs its new co-moving wavelength λ'_{cmf} is given by the standard (non-relativistic) Doppler shift formula

$$\lambda'_{\text{cmf}} = \lambda_{\text{cmf}}(1 + \Delta v/c) \quad (1)$$

where Δv is the change in velocity between the points separated by Δs . In homologous expansion, we have the simple relation⁵ $\Delta v = \Delta s/t$, so the shift in the co-moving frame wavelength $\Delta\lambda_{\text{cmf}} = \lambda'_{\text{cmf}} - \lambda_{\text{cmf}}$ is

$$\Delta\lambda_{\text{cmf}} = \frac{\lambda_{\text{cmf}}}{ct} \Delta s \quad (2)$$

In other words, the comoving wavelength redshifts in *direct proportion* to the distance travelled. This is just like the Hubble expanding universe – photons continually shift to the red.

Assumption 4: We assume the continuum opacity is zero in the line forming region above the photosphere, and consider the opacity of a single line with rest wavelength λ_0 . (We will generalize this to multiple lines below.)

The generic line cross-section is⁶

$$\sigma_l(\lambda) = \left(\frac{\pi e^2}{m_e c} \right) f_{\text{osc}} \phi_\lambda(\lambda) \left(\frac{\lambda_0^2}{c} \right) \quad (3)$$

where f_{osc} is the oscillator strength and ϕ_λ is the line profile. For lines that are intrinsically broadened by thermal Doppler effects, the line profile⁷ $\phi_\lambda \approx 1/\Delta\lambda_T$, where the intrinsic thermal line width is $\Delta\lambda_T = \lambda_0(v_T/c)$, where the thermal velocity $v_T = \sqrt{2k_B T/m}$.

For a typical ejecta temperature $T \approx 10,000$ K and atom mass $m \approx m_p$ the thermal velocities are $v_T \approx 10$ km s⁻¹. This is much less the ejecta expansion velocities $v_{\text{ej}} \approx 10,000$ km s⁻¹, which will permit valuable simplification of the radiation transport.

Assumption 5: The atomic level populations can be calculated in local-thermodynamic equilibrium (LTE). To determine the optical depth of a line, we need to know the number of atoms in the lower level of the atomic transition of interest, as these are the atoms that absorb or scatter light⁸

Consider a transition in a species of atomic number z , an ionization state i , and an excitation state n . In LTE, the number density in the lower level of the transition is

$$\mathcal{N}_{z,i,n} = \frac{\rho X_z}{m_z} f_i \left(\frac{g_n e^{-\Delta E_n/kT}}{\sum_j g_j e^{-\Delta E_j/kT}} \right) \quad (4)$$

⁵ A homogeneously expanding medium is essentially a Hubble-like flow, so every point in the flow looks like it is the center of expansion. Thus, regardless of the direction of the photon, the velocity gradient is $dv/ds = t^{-1}$. In a non-homogeneous flow (e.g., a constant velocity wind) the velocity gradient dv/ds depends on the direction the photon moves – though this is calculable, it complicates the analysis.

⁶ The factor of λ_0^2/c in Eq. 3 appears because we have chosen to define the function ϕ_λ with units of wavelength⁻¹. Had we chosen to define the line profile in frequency space, $\phi_\nu(\nu)$ that factor would not be needed.

⁷ The actual intrinsic line profile for thermal Doppler broadening is given by a Gaussian profile

$$\phi_\lambda = \frac{1}{\sqrt{\pi}\Delta\lambda_T} \exp \left[-\frac{(\lambda - \lambda_0)^2}{\Delta\lambda_T^2} \right]$$

But we will find that the exact line profile shape does not matter and will not worry about this detail here.

⁸ For example, the H_α transition of hydrogen is one from the first excited ($n = 2$) level to the second excited ($n = 3$). Thus, we need to know not just the number density of hydrogen atoms, but the number density of *neutral* hydrogen atoms that are in the $n = 2$ state.

where ρ is the density, X_z is the mass fraction of the species, m_z is the atomic mass of this species, and f_i is the fraction of this atom in the ionization state i . The numerator in parenthesis is the Boltzmann factor that depends on the statistical weight, g_n , and the excitation energy above ground, ΔE_n of the lower level. The denominator in parenthesis is the partition function, i.e., the sum over all levels in the ion which provides the proper normalization⁹.

Assumption 6: We adopt the *Sobolev* (or narrow-line limit) approximation. Consider a line with center wavelength λ_0 and say a photon in the ejecta has co-moving frame wavelength $\lambda_{\text{cmf}} < \lambda_0$. As this photon travels through the ejecta it will not feel the opacity of the line *until* its co-moving frame wavelength has redshifted into *resonance* with the line (i.e., until it achieves $\lambda_{\text{cmf}} \approx \lambda_0$). From Eq. 2, this occurs when the photon has moved a distance

$$\Delta s = (\lambda_0 - \lambda_{\text{cmf}})ct \quad (5)$$

Given that the line has some intrinsic width $\Delta\lambda_T$, the redshifting photon will feel the opacity of the line over some spatial region, called the *resonance region*, which in homologous expansion has a size

$$\Delta l_{\text{res}} = v_t t \quad (6)$$

Since the thermal velocity $v_t \ll v_{\text{ej}}$, we see that the sizes of the resonance region is tiny compared to the size of the ejecta cloud. Thus the resonance region can be taken to be nearly a point.

The essence of the Sobolev approximation is that the properties of the ejecta (i.e., the density, temperature, ionization/excitation state) can be taken to be constant over a resonance region. Thus, a photon's interaction with a line becomes a *local* event, and we can rely only on local properties of the ejecta to determine if a photon interacts with the line at this resonance point.

Problems

Problem 1: Consider a photon that passes through a resonance region. What is the probability that the photon interacts (i.e., is scattered or absorbed) in this region? This is associated with the *Sobolev optical depth*

$$\tau_{\text{sob}} = \int_0^{\Delta l_{\text{res}}} N_{z,i,n} \sigma_l ds \quad (7)$$

⁹ For temperatures T lower than the typical excitation energies, most of the atoms will be in the ground state, and so as a first approximation the partition function is g_0 , where g_0 is the statistical weight of the ground state.

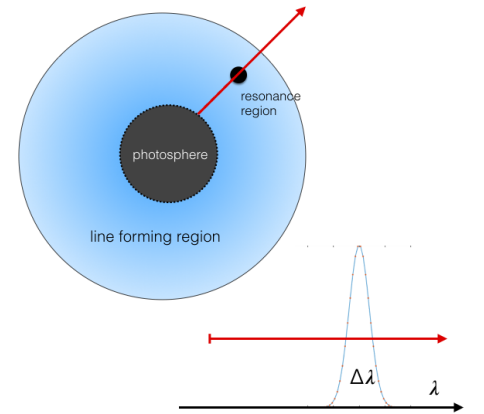


Figure 1: Propagation of a photon (red lines) in an expanding atmosphere. As the photon moves in space, it moves a proportional amount to the red in wavelength. At some point, its comoving frame wavelength can become close to the wavelength of a line λ_0 (i.e., it comes into *resonance* with the line). Because the intrinsic line width is small (thermal velocity $v_T \ll v_{\text{ej}}$) the spatial region where the photon interacts with the line (the *resonance region*) is tiny, essentially a point.

which integrates the line extinction over the spatial dimensions of the resonance region.

1a) Show that the Sobolev optical depth is¹⁰

$$\tau_{\text{sob}} = \left(\frac{\pi e^2}{m_e c} \right) \mathcal{N}_{z,i,n} f_{\text{osc}} \lambda_0 t \quad (9)$$

1b) Show that τ_{sob} of a line is proportional to

$$\tau_{\text{sob}} \propto g_n f_{\text{osc}} \lambda_0 e^{-\Delta E_n / kT} \quad (10)$$

comment: The probability that a photon interacts with a line within its resonance region (i.e., is scatter or absorbed) is simply $1 - e^{-\tau_{\text{sob}}}$. Thus the condition $\tau_{\text{sob}} > 1$ defines a “strong” line. The scaling of Eq. 10 provides a useful wave of estimating which are the important lines in the spectra of supernova or other transients. The [snlines.py](#) code allows you to list lines of different species, sorted by the strength estimated by Eq. 10.

Problem 2: Consider an intensity ray coming off of the photosphere. Solving the radiation transport problem in this case in simple, since the ejecta properties are assumed to be constant over the resonance region. The intensity after passing through a line resonance region is simply

$$I = I_{\text{ph}} e^{-\tau_{\text{sob}}(\vec{r})} + S_{\lambda}(\vec{r})(1 - e^{-\tau_{\text{sob}}(\vec{r})}) \quad (11)$$

where both τ_{sob} and the line source function S_{λ} are evaluated at the resonance region point \vec{r} (which we will see how to locate below). The first term above describes attenuation of the photospheric intensity by the line optical depth, while the second term describes light emitted from the line.

To properly determine the source function S_{λ} requires a full non-LTE solution of the rate equations. However, two approximate methods are useful.

Scattering Line: For a purely scattering line, the line merely redirects the incident radiation field; the source function is $S_{\lambda}(r) = J_{\lambda}(r)$ where J_{λ} averages the intensity coming from all directions.

$$J_{\lambda}(\lambda) = \frac{1}{4\pi} \oint I_{\text{ext}}(\lambda, \theta, \phi) d\Omega \quad (12)$$

where $d\Omega = \sin \theta d\theta d\phi$.

2c) For the case of a spherical photosphere that emits intensity I_{ph} in all directions (see margin figure) show that the $J_{\lambda}(r)$

¹⁰ I am neglecting here the correction for stimulated emission, which in LTE modifies τ_{sob} by a factor

$$\tau_{\text{sob,se}} = \tau_{\text{sob}} (1 - e^{-hc/\lambda_0 kT}) \quad (8)$$

This can be included, though it is a small correction when $hc/\lambda_0 \gg kT$.

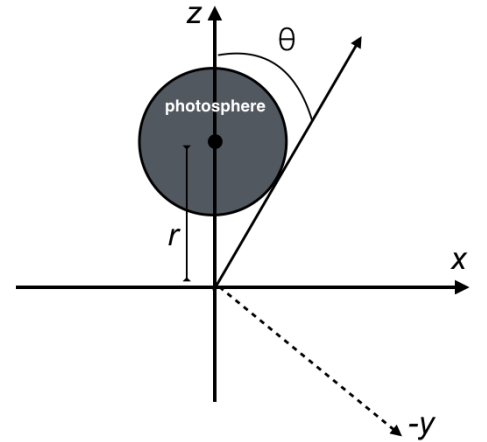


Figure 2: Setup for calculating the mean radiation field $J_{\lambda}(r)$ outside a spherical, constant intensity photosphere. It is convenient to locate the point r at the origin and put the photosphere above on the z -axis.

at a point a distance r from the center is

$$J_\lambda(r) = W(r)I_{\text{ph}} \quad \text{where } W(r) = \frac{1}{2} \left[1 - \sqrt{1 - \frac{R_{\text{ph}}^2}{r^2}} \right] \quad (13)$$

The function $W(r)$ is called the *dilution factor* (as it describes the geometrical dilution of the radiation field).

2d) Take the limits $r = R_{\text{ph}}$ and $r \gg R_{\text{ph}}$ and show that $J_\lambda(r) = W(r)I_{\text{ph}}$ behaves in a reasonable way.

Absorptive line: For purely absorptive lines, the source function is equal to the blackbody function at the local temperature $S_\lambda(r) = B_\lambda(T, r)$.

To estimate the temperature structure, we make the assumption of *radiative equilibrium*, in which at each point in the ejecta radiative heating exactly balances radiative cooling. This is written

$$\oint I_{\text{ph}} \kappa \rho \, d\lambda d\Omega = \oint B_\lambda(T) \kappa \rho \, d\lambda d\Omega \quad (14)$$

where the first term is the heating by photospheric radiation and the second term is cooling by thermal emission. For simplicity, we assume that the incident radiation is solely from the photosphere which emits as a blackbody $I_{\text{ph}} = B_\lambda(T_{\text{ph}})$.

2e) Assume a wavelength-dependent opacity (κ independent of λ) and solve Eq. 14 to determine the temperature $T(r)$ as a function of T_{ph} and r .

Problem 3: Calculate Your Own Supernova Line

TO CALCULATE A SYNTHETIC LINE PROFILE, we must integrate the specific intensity directed towards the observer over the entire ejecta.

It is conventional to define the observer direction to be along the negative- z axis (see Figure 4). Consider a specific intensity ray with observer frame wavelength λ_{obs} directed towards the observer (i.e., parallel to the z axis) at coordinates (x, y) . The ray will come in resonance with the line at the z point

$$z_{\text{res}} = \frac{(\lambda_{\text{obs}} - \lambda_0)}{\lambda_0} ct_{\text{exp}} \quad (15)$$

After passing through the ejecta the specific intensity that is

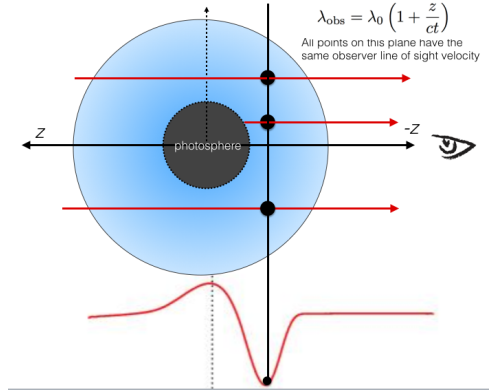


Figure 3: Schematic figure showing that all resonance regions lying along a plane perpendicular to the observer line of sight (the $-z$ direction) map to the same observer wavelength. Thus constructing the observed flux at this wavelength requires integrating up all of these rays using Eq. 16.

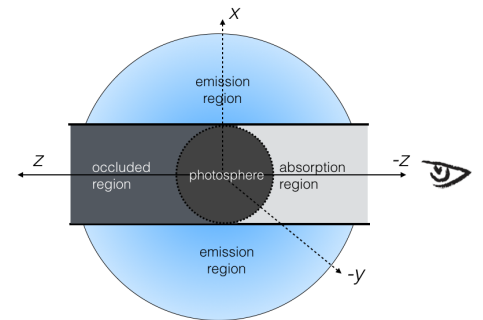


Figure 4: Schematic of line formation in a supernova,

observed will be

$$I(x, y, \lambda_{\text{obs}}) = \begin{cases} I_p e^{-\tau_s} + S(1 - e^{-\tau_s}) & \text{for } p < R_{\text{ph}} \text{ and } r > R_{\text{ph}} \text{ and } z < 0 \text{ (absorption region)} \\ I_p & \text{for } p < R_{\text{ph}} \text{ and } z > 0 \text{ (occluded region)} \\ I_p & \text{for } r < R_{\text{ph}} \text{ (photosphere)} \\ S(1 - e^{-\tau_s}) & \text{for } p > R_{\text{ph}} \text{ (emission region)} \end{cases} \quad (16)$$

where p is the impact parameter $p = \sqrt{x^2 + y^2}$ and the Sobolev optical depth τ_s and source function S_λ should be evaluated at coordinates (x, y, z_{res}) , i.e., the location of the resonance region.

We generate the spectrum by integrating over the rays pointing towards the observer using either Cartesian (x, y, z) or cylindrical polar (z, p, ϕ) coordinates¹¹

$$L_\lambda(\lambda) = \int \int dx dy I(x, y) = \int \int p dp d\phi I(p, \phi) \quad (17)$$

The integral can be extended to the outer edge¹² of the ejecta at some radius $r_{\text{max}} = v_{\text{max}} t_{\text{exp}}$.

3a) Write a code to generate a synthetic line profile by doing the above integral for each value of λ_{obs} you are interested in. To start, you can parameterize the optical depth as $\tau(v) = \tau_0 (v/v_{\text{ph}})^{-m}$ and use the pure scattering line source function.

3b) With your code, analyze how the line profile changes with different values of v_{ph} , τ_0 and the exponent m , and how it is depends on the line source function.

3c) When we have more than one line in the spectrum, we can generalize Eq. 16 and find that

$$I(x, y, \lambda_{\text{obs}}) = \begin{cases} I_p \exp\left(-\sum_{i=1}^N \tau_i\right) + \sum_{i=1}^N S_i (1 - e^{-\tau_i}) \exp\left(-\sum_{j=1}^{i-1} \tau_j\right) & \text{(absorption region)} \\ I_p \exp\left(-\sum_{i=1}^N \tau_i\right) & \text{(occluded region / photosphere)} \\ \sum_{i=1}^N S_i (1 - e^{-\tau_i}) \exp\left(-\sum_{j=1}^{i-1} \tau_j\right) & \text{(emission region)} \end{cases} \quad (18)$$

where the sum over lines runs from bluer lines to redder lines. The τ_{sob} of each line is to be evaluated at the proper z_{es} given by Eq. 15.

3d) Calculate a spectrum including two lines with slightly different line center wavelengths.

3e) Grab the data from the *kurucz_cd23_lines.dat* line list and read in all the lines of a particular species. Using the temperature structure $T(r)$ calculated above, determine the relative

¹¹ Cylindrical-polar coordinates are more convenient for spherical geometries, as the ejecta properties are then independent of ϕ .

¹² Typically one might choose v_{max} to be where the ejecta density has fallen off by a few orders as compared to the photospheric density.

strength of each line (using Eq. 10) and calculate the full spectrum of that ion.

comment: By adding in even more species, you can generalize your code to model an entire spectrum. Given an explosion model, you can thus generate its synthetic spectrum and compare to data. Or if you have an observed spectrum, you may prefer to parameterize $\tau_{\text{sob}}(\vec{r})$ and $S(\vec{r})$ and adjust them until you get a good fit. In the past, such approaches, though quite approximate, have been quite valuable in analyzing data and validating models.