Line Profile Model Derivation, Implementation, and Questions

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Here we present the derivation and implementation of the wind line profile model (Owocki & Cohen 2001):

$$L_x = \frac{C\dot{\mathrm{M}}^2}{2v_\infty^2 R_*}\int_0^{u_{bound}} du \frac{f}{(1-u)^{3\beta}} e^{-\tau[-x/(1-u)^\beta, R_*/u]}.$$

Where f is a filling factor that in principle may be a function of radius but here we'll treat as a constant, while C is an emission normalization constant that in principle contains atomic physics parameters and is proportional to the emissivity. Some of the other variables, including the inverse radial coordinate u and the scaled wavelength x, will be defined below, as will the upper limit of integration.

Changing wind absorption $\tau(p, z)$ into u, x coordinates

If distance from the center of the star is r and θ is the angular coordinate measured from the z-axis which points towards the observer, then $p = r\sin\theta$, and $z = r\cos\theta$. The dummy variable of integration is z' and z is the point we integrate from along a given impact parameter p to obtain the optical depth from the observer to any point in the wind:

$$\tau(p,z) = \begin{cases} \infty, & p \le R_*; z \le \sqrt{{R_*}^2 - p^2} \\ \tau_* \int_z^\infty \frac{R_* dz'}{r'^2(1-R_*/r')^\beta}, & \text{otherwise.} \end{cases}$$

Wind occultation is taken into account by the case of $\tau(p, z) = \infty$.

Since wind absorption is an integral along the z direction, we recast the optical depth integral in cylindrical coordinates and note that for wind photons propagating toward us, p is constant:

$$\tau(p,z) = \tau_* \int_z^\infty \frac{R_* dz'}{(p^2 + z'^2)(1 - R_*/\sqrt{p^2 + z'^2})^\beta}.$$

We now represent the lower bound of integration z and the constant p in terms of $u \equiv R_*/r$ and $x \equiv (\lambda/\lambda_o - 1)c/v_\infty = -v(r)\cos\theta/v_\infty$, the scaled Doppler-shifted wavelength.

The scaled velocity, w, is given by

$$w \equiv \frac{v(r)}{v_\infty}$$

and we therefore have:

$$\frac{z}{r} = \cos\theta = \frac{v_r}{v(r)} = \frac{v_r/v_\infty}{v(r)/v_\infty} = -\frac{x}{w}$$
$$z = -\frac{xr}{w}.$$

Next, we express w and z in terms of u and x, using the beta velocity law:

$$w = \frac{v(r)}{v_\infty} = \frac{v_\infty(1 - \frac{R_*}{r})^\beta}{v_\infty} = (1-u)^\beta$$
$$z = -\frac{xR_*}{u(1-u)^\beta}.$$

For p, we perform a trigonometric conversion:

$$p = \frac{R_*}{u}\sin\theta = \frac{R_*}{u}\sin\left(\cos^{-1}\frac{-x}{(1-u)^\beta}\right) = \frac{R_*\sqrt{(1-u)^{2\beta} - x^2}}{u(1-u)^\beta}.$$

Now, when we perform the optical depth integral, the result will be a function of u and x, so when the full L_x integral is performed over u the result will be a line profile that is explicitly a function of the independent variable, x.

Determining the integration limit of emission line profile

Before we can compute the line profile, we must define some integration limits.

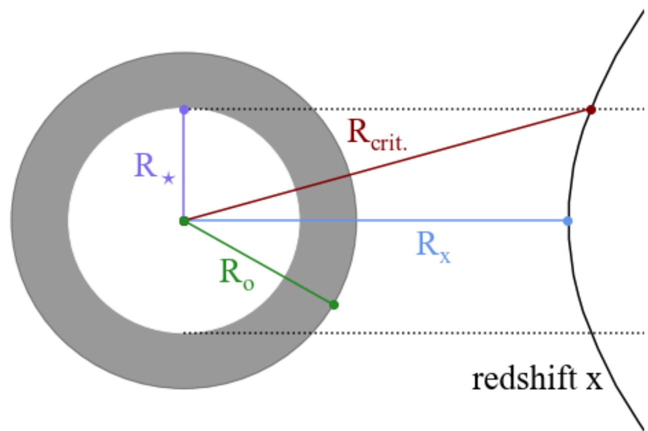

Figure 1: Visualization for the $u_{crit} = R_*/R_{crit}$ derivation. Gray dotted lines represent the boundary of wind occultation. The angle between R_{crit} and R_x is $\pi - \theta$.

Three key parameters are: (1) u_x, which corresponds to the smallest distance from the star on a given x contour, (2) u_o, which is independent x and corresponds to the onset radius of X-ray emission R_o, and (3) u_{crit}, which corresponds to the boundary of wind occultation behind the star on a given x contour[1]. See Fig. 1 for a graphical depiction of these three different quantities.

At u_x, the radial velocity equals the full velocity:

$$|x| = w = (1 - u_x)^\beta$$
$$u_x = 1 - |x|^{1/\beta}.$$

Parameter u_o indicates the onset radius of X-ray emission:

$$u_\mathrm{o} \equiv \frac{R_*}{R_\mathrm{o}}.$$

The value of u_{crit} for a given x is derived using the following procedure, visualized in Fig. 1:

$$x = -\frac{v(R_{crit})\cos\theta}{v_\infty}$$
$$v(R_{crit}) = v_\infty(1 - u_{crit})^\beta$$
$$\cos\theta = -\frac{\sqrt{R_{crit}^2 - {R_*}^2}}{R_{crit}}$$
$$\frac{v_\infty(1 - u_{crit})^\beta\sqrt{R_{crit}^2 - {R_*}^2}}{v_\infty R_{crit}} = x$$
$$(1 - u_{crit})^\beta\sqrt{1 - u_{crit}^2} = x.$$

Now we have defined the three possible boundaries of integration: u_x, u_o, and u_{crit}. The choice of which to use is determined by the following criteria:

$$u_{bound} = \begin{cases} \min\,(u_o, u_x), & x < 0 \\ \min\,(u_o, u_{crit}), & x \geq 0. \end{cases}$$

[1] In Owocki & Cohen (2001), u_x is defined as the minimum of u_o and u_x, but in this document, we use the two distinct labels.

Computing the line profile model

Finally, putting it together, the line profile is computed from:

$$L_x = \frac{C\dot{\mathrm{M}}^2}{2v_\infty^2 R_*} \int_0^{u_{bound}} du \frac{f}{(1-u)^{3\beta}} e^{-\tau_* \int_z^\infty \frac{R_* dz'}{(p^2+z'^2)(1-R_*/\sqrt{p^2+z'^2})^\beta}}$$

where the variables as defined above are $z = -\frac{xR_*}{u(1-u)^\beta}$

and

$$p = \frac{R_* \sqrt{(1-u)^{2\beta} - x^2}}{u(1-u)^\beta}.$$

It can be seen that p will always be real. We note that we evaluate the optical depth integral in cylindrical coordinates, holding p constant and integrating over z'. When evaluating the lower limit of integration, we express z explicitly as a function of x and u.

We show two different combinations of model parameters in Fig. 2, both as a visualization of the line-of-sight velocities and optical depths in a slice of the wind and in Fig. 3 also as line profiles, L_x.

The line profile model is coded in *Python* using *Jupyter Notebook*. Integration is performed with the SciPy *integrate.quad* command inside a for loop over x. We use a single line of code with two nested calls to *integrate.quad* for the whole line profile integral: one integrates the optical depth explicitly in terms of u and x, and the other integrates the emission with respect to u.

We find when evaluating the optical depth integral, where the upper bound of integration is infinity, numerical quadrature integration fails to return plausible results (based on comparisons with Fig. 1 in Owocki & Cohen 2001). Thus, we use a large finite number, $1000\mathrm{R}_*$, rather than infinity, as our upper bound of integration, and produce the models in Fig. 3 that perfectly corresponds to models made with *windprofile* in xspec.

We wonder if another integration method could be used to evaluate this integral exactly, with the upper bound set to infinity. Even with our finite approximation of the integral's upper bound, one model takes of order a minute to run. And so more generally, we wonder if we're solving the optical depth and emission integrals in the most efficient way. We'll note that Owocki & Cohen (2001) state on p. 1111 that the key equation can be "readily evaluated through a single numerical integration," though we are solving them explicitly as two separate integrals, here.

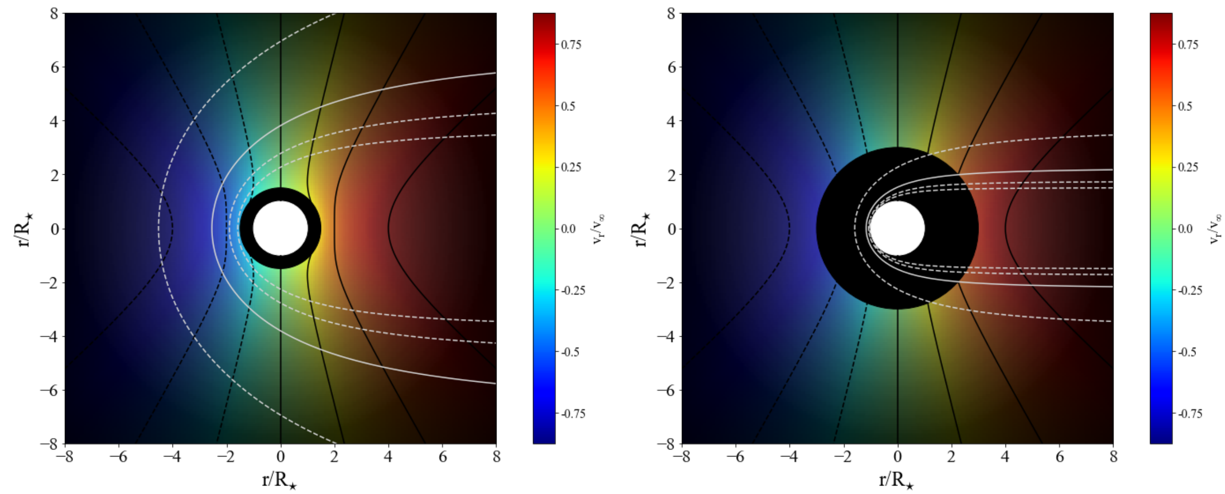

Figure 2: Wind contour model shows the Doppler shift as colored contours enhanced by black contour lines, optical depth in white contour lines (solid line shows where $\tau = 1$, dotted lines are $\tau = 0.5, 1.5,$ and 2), and X-ray emissivity – assumed to scale as the square of the local wind density – as brightness. The figure on the left has $R_{\rm o} = 1.5$, $\tau_* = 2$. The figure on the right has $R_{\rm o} = 3$, $\tau_* = 0.5$.

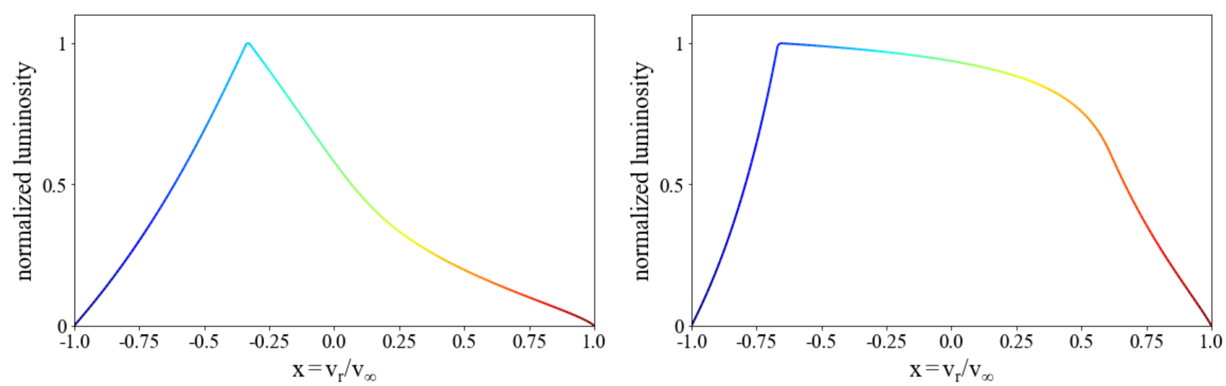

Figure 3: Line profile model, with normalized luminosity over scaled wavelength. Parameters $R_{\rm o}$ and τ_* are the same as in the corresponding panel in Fig. 2.

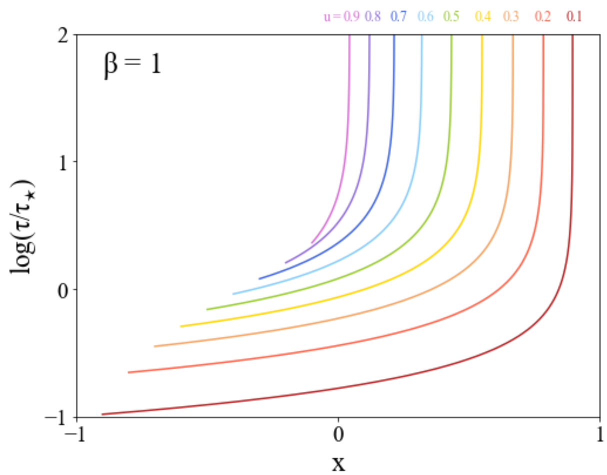

Figure 4: The optical depth, $\log(\tau/\tau_*)$ vs. x, with a range of selected u and a fixed $\beta = 1$. Note that the left-most endpoint of each curve is determined by u_x given by each x.

Model of optical depth vs. scaled wavelength

In the process of figuring out how to solve the optical depth integral, we reproduced the plots in Fig. 1 of Owocki and Cohen (2001) showing the optical depth at select radii as a function of x.

Specifically, we plot $\log(\tau/\tau_*)$ versus scaled wavelength x for a series of u values and a fixed $\beta = 1$ and show the results in Fig. 4. They match the published results well.

For every spherical shell in the wind, namely at each specific u, optical depth can be grouped into three redshift regions (see Fig. 5): (1) large $|x|$ too far from the star to include the u of interest, (2) large x having some contact with u, but the points of contact are within the wind occultation region, and (3) otherwise, where the optical depth is defined and finite.

The first case is exterior to the blue line and its mirrored red line in Fig. 5: $-1 \leq x < x_1; x_3 < x \leq 1$. If the closest point to the star on a given x is bigger than the selected radius, namely if $u_x < u$, then u does not intersect with that x contour at all, and optical depth is undefined. The boundary cases are given by:

$$u_x = u$$
$$|x| = (1-u)^{\beta}.$$

The second case is represented by the region between the green and the red lines in Fig. 5: $x_2 \leq x \leq x_3$, $u_{crit} \leq u \leq u_x$. This is when x intersects with u but the intersection is within the wind occultation region. The boundary case for occultation is:

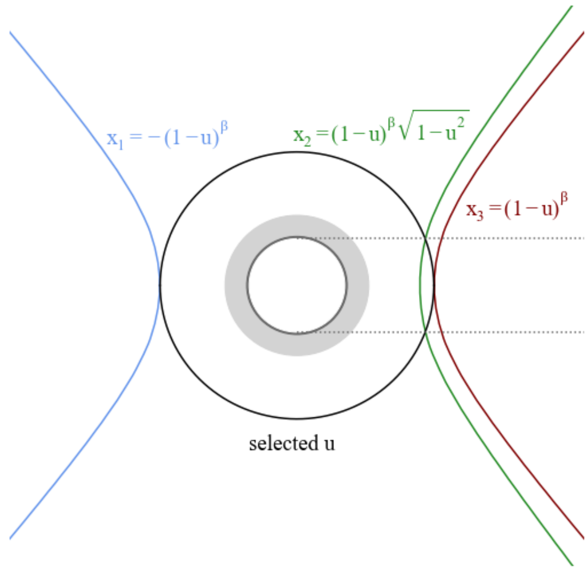

Figure 5: Visualization for the boundaries of x that specifies the three regions where τ is defined differently.

$$u = u_{crit}$$
$$(1-u)^\beta\sqrt{1-u^2} = x$$

The third case is represented by the region between the blue and the green lines in Fig. 5: $x_1 \leq x < x_2$, which has a finite optical depth.

Thus, the log of the scaled optical depth over scaled wavelength on a selected u is given by the following equation:

$$\log\left(\tau/\tau_*\right) = \begin{cases} \text{undefined}, & u_x < u \\ \infty, & u_{crit} \leq u \leq u_x; x \geq 0 \\ \log\int_z^\infty \frac{R_* dz'}{(p^2+z'^2)(1-R_*/\sqrt{p^2+z'^2})^\beta}, & \text{otherwise} \end{cases}$$

When plotting the optical depth model in Fig. 4, we again set the upper bound of integration to $1000R_*$ due to our problems with *integrate.quad*. To fully evaluate the optical depth contours, we required up to 20,000 points on x, and the calculation took about four minutes to run. This also makes us wonder if there is a more efficient way to calculate the optical depth.