

Radiative Transfer Equation for Cloudy Atmospheres

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1 Definitions

As radiation makes its way through the atmosphere, it may be weakened by **absorption** and **scattering**. The combined effect of absorption and scattering is called **extinction**.

Attenuation, α

Attenuation, or **extinction**, is the gradual loss in intensity of any kind of flux through a medium. For instance, sunlight is attenuated by dark glasses, X-rays are attenuated by lead, and light and sound are attenuated while passing through water. Attenuation affects the propagation of waves and signals in electrical circuits, in optical fibers, as well as in air.

In many cases, attenuation is an exponential function of the path length through the medium. In chemical spectroscopy, this is known as the Beer-Lambert law.

In engineering, attenuation is usually measured in units of decibels per unit length of medium (dB/cm, dB/km, etc.) and is represented by the attenuation coefficient of the medium in question.

Absorption Cross Section, β

Absorption cross section is a measure for the probability of an absorption process. Absorption cross section is the ability of a molecule to absorb a photon of a particular wavelength (and polarization).

The **absorption cross section** C_a is defined as the ratio of *absorbed power* P_a to the *incident power density*.

The **absorption efficiency** ξ_a is defined as the ratio of C_a to the particle cross-section-area A . For a spherical particle of radius r , we have $\xi_a = \frac{C_a}{\pi r^2}$.

The **scattering cross section** C_s is defined as the ratio of *scattered power* P_s to the *incident power density*.

The **scattering efficiency** ξ_s is defined as the ratio C_s to the particle cross-section-area A . For a spherical particle of radius r , we have $\xi_s = \frac{C_s}{\pi r^2}$.

The sum of ξ_a and ξ_s is the **extinction efficiency** $\xi_e = \xi_a + \xi_s$.

Beer-Lambert Law

In optics, the **Beer-Lambert law** relates the absorption of light to the properties of the material through which the light is traveling.

The law states that there is a logarithmic dependence between the transmission (or transmissivity), \mathcal{T} , of light through a substance and the product of the absorption coefficient of the substance, α , and the distance the light travels through the material (i.e. the path length), s . The absorption coefficient can, in turn, be written as a product of an absorption cross section, β , and the (number) density F of absorbers.

These relations can be written as

$$\mathcal{T} = \frac{I}{I_0} = e^{-\alpha s} = e^{-\beta F s}.$$

where I_0 and I are the intensity (or power) of the incident light and the transmitted light, respectively; β is cross section of light absorption by a single particle and F is the density (number per unit volume) of absorbing particles.

Black Body

Planck's law describes the spectral radiance of electromagnetic radiation at all wavelengths emitted in the normal direction from a black body in a cavity in thermodynamic equilibrium. The source function is a characteristic of a stellar atmosphere, and in the case of no scattering of photons, describes the ratio of the emission coefficient to the absorption coefficient.

A black body is an object that absorbs all light that falls on it, and emits light in a wavelength spectrum determined solely by its temperature.

The emissivity of a material (usually written ϵ or e) is the relative ability of its surface to emit energy by radiation. It is the ratio of energy radiated by a particular material to energy radiated by a black body at the same temperature. It is a measure of a material's ability to radiate absorbed energy. A true black body would have an $\epsilon = 1$ while any real object would have $\epsilon < 1$. Emissivity is a dimensionless quantity, so it does not have units.

In general, the duller and blacker a material is, the closer its emissivity is to 1. The more reflective a material is, the lower its emissivity. Highly polished silver has an emissivity of about 0.02.

When dealing with non-black surfaces, the deviations from ideal black body behavior are determined by both the geometrical structure and the chemical composition, and follow Kirchhoff's law of thermal radiation: emissivity equals absorptivity (for an object in thermal equilibrium), so that an object that does not absorb all incident light will also emit less radiation than an ideal black body.

Total single scattering albedo, ω_0 , is a quantity reflecting the relative importance of cloud scattering in a background atmosphere. It is defined as the ratio of cloud volume scattering β_{c-s} and the total volume extinction β_e :

$$\omega_0 = \frac{\beta_{c-s}}{\beta_e}. \quad (1)$$

The area element on the sphere is given in *spherical coordinates* by $dA = r^2 \sin \theta d\theta d\phi$. The total area can thus be obtained by integration:

$$A = \int_0^{2\pi} \int_0^\pi r^2 \sin \theta d\theta d\phi = 4\pi r^2.$$

2 The Generalized Radiative Transfer Equation

The radiative process is described by the generalized radiative transfer equation:

$$\frac{dI}{ds} = -\beta_e I + \beta_a B + \beta_s J_s,$$

where

β_{gas_a}	gas volume absorption coefficient,
β_{c_s}	cloud volume scattering coefficient,
β_{c_a}	cloud volume absorption coefficient,
$\beta_e = \beta_{gas_a} + \beta_{c_s} + \beta_{c_a}$	total volume extinction coefficient,
$\beta_a = \beta_{gas_a} + \beta_{c_a}$	total volume absorption coefficient,
$\beta_s = \beta_{c_s}$	total volume scattering coefficient.

One way to derive this equation is to consider the radiative transfer equation for a *nonscattering* atmosphere:

$$\frac{\partial I}{\partial s} = -\beta_e I + \beta_e B, \quad (2)$$

and to replace B with $\bar{B} = (1 - \omega_0)B + \omega_0 T_{\text{scat}}$, where ω_0 is defined in (1):

$$\begin{aligned}\frac{\partial I}{\partial s} &= -\beta_e I + \beta_e \bar{B} \\ &= -\beta_e I + \beta_e (1 - \omega_0)B + \beta_e \omega_0 T_{\text{scat}} \\ &= -\beta_e I + (\beta_e - \beta_s)B + \beta_s T_{\text{scat}} \\ &= -\beta_e I + \beta_a B + \beta_s T_{\text{scat}}.\end{aligned}$$

2.1 Alternate form of radiative transfer equation

Starting with:

$$\begin{aligned}\frac{dI}{ds} + \beta_e I &= \beta_a B + \beta_s J_s, \\ \frac{1}{\beta_e} \frac{dI}{ds} + I &= \frac{\beta_a}{\beta_e} B + \frac{\beta_s}{\beta_e} J_s, \\ \frac{1}{\beta_e} \frac{dI}{ds} + I &= \left(1 - \frac{\beta_{c-s}}{\beta_e}\right) B + \frac{\beta_{c-s}}{\beta_e} J_s, \\ \frac{1}{\beta_e} \frac{dI}{ds} + I &= (1 - \omega_0) B + \omega_0 J_s.\end{aligned}$$

2.2 Efficiency Factors

The **absorption cross section** C_a is defined as the ratio of *absorbed power* P_a to the *incident power density*.

The **absorption efficiency** ξ_a is defined as the ratio of C_a to the particle cross-section-area A . For a spherical particle of radius r , we have

$$\xi_a = \frac{C_a}{\pi r^2}.$$

The **scattering cross section** C_s is defined as the ratio of *scattered power* P_s to the *incident power density*.

The **scattering efficiency** ξ_s is defined as the ratio C_s to the particle cross-section-area A . For a spherical particle of radius r , we have

$$\xi_s = \frac{C_s}{\pi r^2}.$$

The sum of ξ_a and ξ_s is the **extinction efficiency** ξ_e :

$$\xi_e = \xi_a + \xi_s.$$

2.3 Scattering Phase Function

The angular distribution of the scattered light is represented by a phase function $P(\theta)$, where θ is the scattering solid angle (the difference between the solid angle of scattered radiation and incident radiation). The phase function is normalized such that its integral over all angles is 4π , that is,

$$\frac{1}{4\pi} \oint P(\theta, \theta') d\theta' = 1.$$

2.4 Particle Size Parameter

The particle size parameter χ is defined as the ratio of the circumference of a spherical particle to the wavelength:

$$\chi = \frac{2\pi r}{\lambda}.$$

2.5 Mie Efficiencies

The Mie solution gives the scattering and extinction efficiencies [26] (Section 4.4.2.1), [7, 8, 9]¹
²:

$$\begin{aligned}\xi_s &= \frac{2}{\chi^2} \sum_{n=1}^{n_{\text{cut}}} (2n+1)(|a_n|^2 + |b_n|^2), \\ \xi_e &= \frac{2}{\chi^2} \sum_{n=1}^{n_{\text{cut}}} (2n+1) [\Re(a_n)^2 + \Im(a_n)^2 + \Re(b_n)^2 + \Im(b_n)^2], \\ \xi_e &= \frac{2}{\chi^2} \sum_{n=1}^{n_{\text{cut}}} (2n+1) \Re(a_n + b_n),\end{aligned}$$

where a_n and b_n are complex Mie coefficients [6]:

$$a_n = \frac{(A_n/m + n/\chi)\Re(W_n) - \Re(W_{n-1})}{(A_n/m + n/\chi)W_n - W_{n-1}}, \quad (3)$$

$$b_n = \frac{(mA_n + n/\chi)\Re(W_n) - \Re(W_{n-1})}{(mA_n + n/\chi)W_n - W_{n-1}}. \quad (4)$$

Intermediate variables W_n and A_n are calculated from the recursive expressions: ³

$$W_n = \left(\frac{2n-1}{\chi} \right) W_{n-1} - W_{n-2},$$

where

$$W_0 = \sin \chi + i \cos \chi,$$

$$W_{-1} = \cos \chi - i \sin \chi,$$

and ⁴

$$\begin{aligned}A_n &= -\frac{n}{m\chi} + \left(\frac{n}{m\chi} - A_{n-1} \right)^{-1}, \\ A_0 &= \cot m\chi.\end{aligned}$$

The complex refractive index m is given as

$$m = \sqrt{\varepsilon},$$

where ε is the complex dielectric constant [26] (Section 4.4.1.2 and Appendix C) with

$$\begin{aligned}\Re(\varepsilon) &= 3.15, \\ \Im(\varepsilon) &= \alpha(T)/\nu + \beta(T)\nu,\end{aligned}$$

where ν is frequency in GHz, and the temperature dependent parameters $\alpha(T)$ and $\beta(T)$ are given in [26] (Appendix C).

¹Section 5 in [8] is obsolete.

² ξ_s and ξ_e are computed by Mie_efficiencies.

³wvs-058 derives and wvs-065,wvs-066,wvs-067 present expressions for A_n and W_n in terms of Bessel and Hankel functions.

⁴Note that an equivalent relation to forward recurrence $A_n(m\chi) = -\frac{n}{m\chi} + \left(\frac{n}{m\chi} - A_{n-1}(m\chi) \right)^{-1}$ is backward recurrence $A_{n-1}(m\chi) = \frac{n}{m\chi} - \left(\frac{n}{m\chi} + A_n(m\chi) \right)^{-1}$, which is used in sphbes.f90.

Intermediate variables in terms of Bessel functions

Using notations for spherical Bessel functions in Appendix 8, rewrite

$$W_n = \left(\frac{2n-1}{\chi} \right) W_{n-1} - W_{n-2},$$

where

$$W_0 = \chi h_0^{(2)}(\chi) = \chi (j_0(\chi) - iy_0(\chi)),$$

$$W_{-1} = \chi h_{-1}^{(2)}(\chi) = \chi (j_{-1}(\chi) - iy_{-1}(\chi)).$$

From Appendix 8, we have

$$h_{n-2}(\chi) + h_n(\chi) = \left(\frac{2n-1}{\chi} \right) h_{n-1}(\chi).$$

Multiply by χ :

$$\chi h_{n-2}(\chi) + \chi h_n(\chi) = \left(\frac{2n-1}{\chi} \right) \chi h_{n-1}(\chi).$$

or

$$W_{n-2} + W_n = \left(\frac{2n-1}{\chi} \right) W_{n-1}.$$

2.6 Phase function

Since the intensity of the scattered radiation is proportional to the sum of the square of two amplitude functions $S_1(\theta, r, T)$ and $S_2(\theta, r, T)$ for electric fields perpendicular and parallel to the plane of scattering, respectively, the phase function can be written as [26] (Section 4.4.2.2), [7, 10, 11]:

$$p(\theta, r, T) = \frac{p_0(\theta, r, T)}{C(r, T)} \quad (5)$$

where

$$\begin{aligned} p_0(\theta, r, T) &= |S_1(\theta, r, T)|^2 + |S_2(\theta, r, T)|^2 \\ &= \Re(S_1(\theta, r, T))^2 + \Im(S_1(\theta, r, T))^2 + \Re(S_2(\theta, r, T))^2 + \Im(S_2(\theta, r, T))^2, \end{aligned} \quad (6)$$

and the normalization function is

$$C(r, T) = \frac{1}{2} \int_0^\pi p_0(\theta, r, T) \sin \theta d\theta. \quad (7)$$

The Mie solution for the two amplitude functions is given by ⁵

$$\begin{aligned} S_1(\theta, r, T) &= \sum_{j=1}^{\infty} \frac{2j+1}{j(j+1)} \left(a_j(r, T) \frac{dP_j^1(\cos \theta)}{d\theta} + b_j(r, T) \frac{P_j^1(\cos \theta)}{\sin \theta} \right), \\ S_2(\theta, r, T) &= \sum_{j=1}^{\infty} \frac{2j+1}{j(j+1)} \left(a_j(r, T) \frac{P_j^1(\cos \theta)}{\sin \theta} + b_j(r, T) \frac{dP_j^1(\cos \theta)}{d\theta} \right), \end{aligned}$$

⁵ a_j and b_j are functions of r through χ and are functions of T through ε .

where a_j and b_j are the Mie coefficients defined by equations (3) and (4).⁶

The quantities P_j^1 are the associated Legendre polynomials, which are derived from the recurrence relations. Given the initial values $P_1^1 = \sin \theta$ and $P_2^1 = 3 \cos \theta \sin \theta$, the subsequent polynomials and the corresponding derivatives are given as⁷

$$\begin{aligned} P_j^1 &= \left(\frac{2j-1}{j-1} \right) P_{j-1}^1 \cos \theta - \left(\frac{j}{j-1} \right) P_{j-2}^1, \\ \frac{dP_j^1}{d\theta} &= \left(\frac{2j-1}{j-1} \right) \left(\cos \theta \frac{dP_{j-1}^1}{d\theta} - P_{j-1}^1 \sin \theta \right) - \left(\frac{j}{j-1} \right) \frac{dP_{j-2}^1}{d\theta}. \end{aligned}$$

2.6.1 Derivatives of Phase Function

From equation (6) defining p_0 , we have [10]:

$$\begin{aligned} \frac{\partial p_0(\theta, r, T)}{\partial T} &= \frac{\partial}{\partial T} (\Re(S_1(\theta, r, T))^2 + \Im(S_1(\theta, r, T))^2 + \Re(S_2(\theta, r, T))^2 + \Im(S_2(\theta, r, T))^2) \\ &= 2 \left(\Re(S_1(\theta, r, T)) \frac{\partial \Re(S_1(\theta, r, T))}{\partial T} + \Im(S_1(\theta, r, T)) \frac{\partial \Im(S_1(\theta, r, T))}{\partial T} \right. \\ &\quad \left. + \Re(S_2(\theta, r, T)) \frac{\partial \Re(S_2(\theta, r, T))}{\partial T} + \Im(S_2(\theta, r, T)) \frac{\partial \Im(S_2(\theta, r, T))}{\partial T} \right). \end{aligned}$$

Taking the derivative of the phase function p in equation (5) with respect to temperature T and using (7), we have

$$\begin{aligned} \frac{\partial p(\theta, r, T)}{\partial T} &= \frac{\partial}{\partial T} \left(\frac{p_0(\theta, r, T)}{C(r, T)} \right) \\ &= \frac{1}{C(r, T)^2} \left(\frac{\partial p_0(\theta, r, T)}{\partial T} C(r, T) - p_0(\theta, r, T) \frac{\partial C(r, T)}{\partial T} \right) \\ &= \frac{1}{C(r, T)} \left(\frac{\partial p_0(\theta, r, T)}{\partial T} - \frac{p_0(\theta, r, T)}{C(r, T)} \frac{\partial C(r, T)}{\partial T} \right) \\ &= \frac{1}{C(r, T)} \left(\frac{\partial p_0(\theta, r, T)}{\partial T} - p(\theta, r, T) \frac{\partial C(r, T)}{\partial T} \right) \\ &= \frac{1}{C(r, T)} \left(\frac{\partial p_0(\theta, r, T)}{\partial T} - \frac{p(\theta, r, T)}{2} \int_0^\pi \frac{\partial p_0(\theta, r, T)}{\partial T} \sin \theta d\theta \right). \end{aligned}$$

Since $a_j(r, T)$ and $b_j(r, T)$ are not functions of ice water content \mathcal{I} , the derivative of the phase function with respect to \mathcal{I} is 0:

$$\frac{\partial p(\theta, r, T)}{\partial \mathcal{I}} = 0. \tag{8}$$

2.7 Volume Scattering and Extinction Coefficients

The total cloud extinction coefficient is a direct summation of all the individual particle contributions, [26] (Section 4.4.3.1), [7, 8, 9, 12] i.e.⁸

$$\beta_{c-e} = \pi \int_0^\infty n(r) r^2 \xi_e(r) dr.$$

⁶Here, P_j^1 are presumed to be functions of $\cos \theta$. It is true for expressions in wvs-068. It is not true for what is here and in Cloud ATBD (P_1^1 is not a function of $\cos \theta$).

⁷These are equations (4.42) and (4.43) from [26]. In wvs-068, equations are different.

⁸Note that in some documents (e.g. wvs-066), there is a factor of 2π instead of π .

The total cloud scattering coefficient is given by

$$\beta_{c_s} = \pi \int_0^\infty n(r) r^2 \xi_s(r) dr.$$

The total volume absorption coefficient is given by

$$\beta_{c_a} = \beta_{c_e} - \beta_{c_s}.$$

2.7.1 McFarquhar-Heymsfield (MH) Distribution

The McFarquhar and Heymsfield particle-size distribution function $n(r)$ is composed of a first-order gamma distribution function for small particles ($D < 100\mu\text{m}$) and log-normal distribution function for large particles ($D > 100\mu\text{m}$), and is given by [2], [26] (Section 5.3.2.1 and Appendix E1), [7, 8, 9, 12]⁹:

$$n(r) = N_1 2r \exp(-\alpha 2r) + \frac{N_2}{2r} \exp \left[-\frac{1}{2} \left(\frac{\log(2r/D_0) - \mu}{\sigma} \right)^2 \right],$$

where¹⁰

$$N_1 = \frac{\mathcal{I}_{<100} \alpha^5}{4\pi\rho_{\text{ice}}}, \quad (9)$$

$$N_2 = \frac{6}{\sqrt{2\pi^3} \rho_{\text{ice}} D_0^3 \sigma} \frac{\mathcal{I}_{>100}}{\exp(3\mu + 4.5\sigma^2)}, \quad (10)$$

and $D_0 = 1 \mu\text{m}$, $\rho_{\text{ice}} = 0.91 \text{ g/m}^3$.

The quantities $\mathcal{I}_{<100}$ and $\mathcal{I}_{>100}$ are the total ice content of particles with $D < 100\mu\text{m}$ and $D > 100\mu\text{m}$, respectively. They are calculated from parameters α , μ , and σ for a given \mathcal{I} . These parameters are defined as¹¹

$$\begin{aligned} \mathcal{I}_{<100} &= \min[\mathcal{I}, 0.252(\mathcal{I}/\mathcal{I}_0)^{0.837}], \\ \mathcal{I}_{>100} &= \mathcal{I} - \mathcal{I}_{<100}, \\ \alpha &= -4.99 \times 10^{-3} - 0.0494 \log_{10}(\mathcal{I}_{<100}/\mathcal{I}_0), \\ \mu &= (5.2 + 0.0013T) + (0.026 - 1.2 \times 10^{-3}T) \log_{10}(\mathcal{I}_{>100}/\mathcal{I}_0), \\ \sigma &= (0.47 + 2.1 \times 10^{-3}T) + (0.018 - 2.1 \times 10^{-4}T) \log_{10}(\mathcal{I}_{>100}/\mathcal{I}_0). \end{aligned} \quad (11)$$

\mathcal{I} is the ice water content of the atmosphere in g/m^3 , $\mathcal{I}_0 = 1 \text{ g/m}^3$, and T is the atmospheric temperature in Celcius.¹²

Note that N_2, μ, σ depend on both temperature T and ice water content \mathcal{I} , and N_1, α depend on ice water content \mathcal{I} , but not on temperature T :

$$\frac{\partial \alpha}{\partial T} = \frac{\partial N_1}{\partial T} = 0.$$

None of these quantities depend on θ nor r [12].

⁹More details are given in the references above. Note that in [26] (Appendix E1), $n(D)$ is given as two expressions, while in ATBD [26] (Section 5.3.2.1), wvs-065,wvs-066,wvs-067,wvs-071, it is expressed as summation, similar to here.

¹⁰Equation (5.3) in ATBD [26] has an exponent of 1, not 3, for D_0 in the denominator of the expression for N_2 in Equation (10). In Equation (4) in [2], the exponent is 3.

¹¹Equation (5.6) in ATBD [26] has +0.0494 in the expression for α in Equation (11). Equation (6) in [2] has -0.0494.

¹²Tables 1 and 2 on page 2193 in [2] give coefficients as a function of degrees Celsius.

2.7.2 IWC Derivatives

Since $\mathcal{I}_{<100} = \min[\mathcal{I}, 0.252(\mathcal{I}/\mathcal{I}_0)^{0.837}]$, there are two cases to consider.

Case 1: $\mathcal{I} \leq 0.252(\mathcal{I}/\mathcal{I}_0)^{0.837}$. Therefore, $\mathcal{I}_{<100} = \mathcal{I}$ and $\mathcal{I}_{>100} = \mathcal{I} - \mathcal{I}_{<100} = 0$. From equations (9), (10), and (11):¹³

$$\begin{aligned}\frac{\partial \alpha}{\partial \mathcal{I}} &= -\frac{0.0494}{\mathcal{I} \ln 10} = -\frac{0.02145}{\mathcal{I}}, \\ \frac{\partial N_1}{\partial \mathcal{I}} &= \frac{1}{4\pi\rho_{\text{ice}}} \frac{\partial}{\partial \mathcal{I}} (\mathcal{I} \alpha^5) = \frac{1}{4\pi\rho_{\text{ice}}} \left(\alpha^5 + 5\mathcal{I}\alpha^4 \frac{\partial \alpha}{\partial \mathcal{I}} \right), \quad \text{or} \\ \frac{1}{N_1} \frac{\partial N_1}{\partial \mathcal{I}} &= \frac{1}{\mathcal{I}} + \frac{5}{\alpha} \frac{\partial \alpha}{\partial \mathcal{I}},\end{aligned}$$

Case 2: $\mathcal{I} > 0.252(\mathcal{I}/\mathcal{I}_0)^{0.837}$. Therefore, $\mathcal{I}_{<100} = 0.252(\mathcal{I}/\mathcal{I}_0)^{0.837}$ and $\mathcal{I}_{>100} = \mathcal{I} - \mathcal{I}_{<100}$.

Plotting \mathcal{I} and $0.252(\mathcal{I}/\mathcal{I}_0)^{0.837}$ as functions of \mathcal{I} with $\mathcal{I}_0 = 1 \text{ g/m}^3$, we see that for Case 1, $\mathcal{I} < 2.1262 \times 10^{-4}$, and for Case 2, $\mathcal{I} > 2.1262 \times 10^{-4}$.

2.8 The Integrated Phase Function

The integrated phase function is computed by summing up all the individual phase functions from the Mie calculations and weighing each one by its scattering efficiency $\pi r^2 \xi_s$ [26] (Section 4.4.3.2),[9, 12]:

$$P(\theta) = \frac{\pi}{\beta_{c,s}} \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr, \quad (12)$$

where θ is the scattering angle.

2.8.1 Derivatives of the Integrated Phase Function

The derivative of the integrated phase function P in (12) with respect to temperature is [10]:

$$\begin{aligned}\frac{\partial P(\theta)}{\partial T} &= \frac{\partial}{\partial T} \left(\frac{\pi}{\beta_{c,s}} \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \right) \\ &= \frac{\pi}{\beta_{c,s}} \frac{\partial}{\partial T} \left(\int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \right) + \frac{\partial}{\partial T} \left(\frac{\pi}{\beta_{c,s}} \right) \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \\ &= \frac{\pi}{\beta_{c,s}} \int_0^\infty r^2 \left(\frac{\partial n(r)}{\partial T} \xi_s(r) p(\theta, r) + n(r) \frac{\partial \xi_s(r)}{\partial T} p(\theta, r) + n(r) \xi_s(r) \frac{\partial p(\theta, r)}{\partial T} \right) dr \\ &\quad - \frac{\pi}{\beta_{c,s}^2} \frac{\partial \beta_{c,s}}{\partial T} \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \\ &= \frac{\pi}{\beta_{c,s}} \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) \left(\frac{1}{n(r)} \frac{\partial n(r)}{\partial T} + \frac{1}{\xi_s(r)} \frac{\partial \xi_s(r)}{\partial T} + \frac{1}{p(\theta, r)} \frac{\partial p(\theta, r)}{\partial T} \right) dr \\ &\quad - \frac{P(\theta)}{\beta_{c,s}} \frac{\partial \beta_{c,s}}{\partial T}.\end{aligned}$$

¹³ $\frac{d}{dx} \log_b(x) = \frac{d}{dx} \left(\frac{1}{\ln(b)} \ln x \right) = \frac{1}{\ln(b)} \frac{d}{dx} \ln x = \frac{1}{x \ln(b)}$.

Geometry of Discrete Radiative Transfer

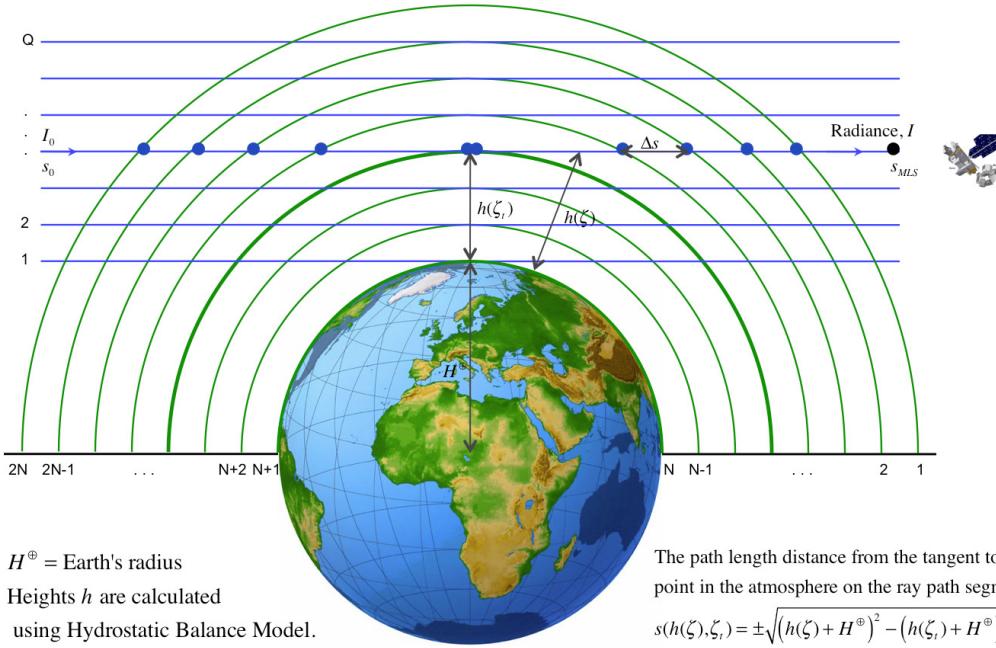


Figure 1: Geometry of discrete radiative transfer

Considering equations (8) and (13) the derivative of the integrated phase function P in (12) with respect to ice water content is [10]:¹⁴

$$\begin{aligned} \frac{\partial P(\theta)}{\partial \mathcal{I}} &= \frac{\partial}{\partial \mathcal{I}} \left(\frac{\pi}{\beta_{c,s}} \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \right) \\ &= \frac{\pi}{\beta_{c,s}} \frac{\partial}{\partial \mathcal{I}} \left(\int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \right) + \frac{\partial}{\partial \mathcal{I}} \left(\frac{\pi}{\beta_{c,s}} \right) \int_0^\infty r^2 n(r) \xi_s(r) p(\theta, r) dr \\ &= \frac{\pi}{\beta_{c,s}} \int_0^\infty r^2 \frac{\partial n(r)}{\partial \mathcal{I}} \xi_s(r) p(\theta, r) dr - \frac{P(\theta)}{\beta_{c,s}} \frac{\partial \beta_{c,s}}{\partial \mathcal{I}}. \end{aligned}$$

The derivatives of $n(r)$ with respect to temperature T and ice water content \mathcal{I} are given in [8].

3 Discrete Radiative Transfer Equation

See Figure 1 for geometry of discrete radiative transfer.

¹⁴The derivatives of P in wvs-065 and wvs-067 are derived from a $P(\theta)$ written as a single integral version (unlike what was done here and in wvs-068).

3.1 Nonscattering Atmosphere

For *nonscattering* atmosphere, the radiative transfer equation is

$$\begin{aligned} I(\mathbf{x}) &= \sum_{i=1}^{2N} \Delta B_i \mathcal{T}_i = \Delta B_1 \mathcal{T}_1 + \Delta B_2 \mathcal{T}_2 + \dots + \Delta B_{2N-1} \mathcal{T}_{2N-1} + \Delta B_{2N} \mathcal{T}_{2N} \\ &\approx - \int_{B(s_0)}^{B(s_{\mathfrak{M}})} \mathcal{T}(s) dB(s) + (I(s_0) - B(s_0)) \mathcal{T}(s_0) + B(s_{\mathfrak{M}}), \end{aligned}$$

where

$$\begin{aligned} \Delta B_1 &= \frac{B_1 + B_2}{2} \approx B(s_{\mathfrak{M}}), \\ \Delta B_i &= \frac{B_{i+1} - B_{i-1}}{2}, \\ \Delta B_{2N} &= I_0 - \frac{B_{2N-1} + B_{2N}}{2} \approx I(s_0) - B(s_0). \end{aligned}$$

3.2 Scattering Atmosphere

For *scattering* atmosphere, the radiative transfer equation is [22]

$$\begin{aligned} I(\mathbf{x}) &= \sum_{i=1}^{2N} \Delta \bar{B}_i \mathcal{T}_i = \Delta \bar{B}_1 \mathcal{T}_1 + \Delta \bar{B}_2 \mathcal{T}_2 + \dots + \Delta \bar{B}_{2N-1} \mathcal{T}_{2N-1} + \Delta \bar{B}_{2N} \mathcal{T}_{2N} \\ &\approx - \int_{\bar{B}(s_0)}^{\bar{B}(s_{\mathfrak{M}})} \mathcal{T}(s) d\bar{B}(s) + (I(s_0) - \bar{B}(s_0)) \mathcal{T}(s_0) + \bar{B}(s_{\mathfrak{M}}), \end{aligned}$$

where

$$\bar{B} = (1 - \omega_0)B + \omega_0 T_{\text{scat}},$$

and

$$\begin{aligned} \Delta \bar{B}_i &= \frac{\bar{B}_{i+1} - \bar{B}_{i-1}}{2} \\ &= \frac{1}{2} \left((1 - \omega_{0,i+1})B_{i+1} + \omega_{0,i+1}T_{\text{scat},i+1} - (1 - \omega_{0,i-1})B_{i-1} - \omega_{0,i-1}T_{\text{scat},i-1} \right) \\ &= \frac{1}{2} \left([(1 - \omega_{0,i+1})B_{i+1} - (1 - \omega_{0,i-1})B_{i-1}] + [\omega_{0,i+1}T_{\text{scat},i+1} - \omega_{0,i-1}T_{\text{scat},i-1}] \right) \\ &= \Delta \bar{B}_i^g + \Delta \bar{B}_i^s, \end{aligned}$$

where $\Delta \bar{B}_i^g$ and $\Delta \bar{B}_i^s$ are **gas** and **scattering** parts, respectively.

For $i = 2, \dots, 2N-1$, we have

$$\begin{aligned} \Delta \bar{B}_i^g &= \frac{1}{2} \left((1 - \omega_{0,i+1})B_{i+1} - (1 - \omega_{0,i-1})B_{i-1} \right) \quad \text{and} \\ \Delta \bar{B}_i^s &= \frac{1}{2} \left(\omega_{0,i+1}T_{\text{scat},i+1} - \omega_{0,i-1}T_{\text{scat},i-1} \right). \end{aligned}$$

At one end of the path, closest to the instrument (for $i = 1$), we have

$$\begin{aligned} \Delta \bar{B}_1^g &= \frac{1}{2} ((1 - \omega_{0,1})B_1 + (1 - \omega_{0,2})B_2), \\ \Delta \bar{B}_1^s &= \frac{1}{2} (\omega_{0,1}T_{\text{scat},1} + \omega_{0,2}T_{\text{scat},2}). \end{aligned}$$

At another end of the path, farther away from the instrument (for $i = 2N$), we have

$$\begin{aligned} \Delta \bar{B}_{2N}^g &= I_0 - \frac{1}{2} ((1 - \omega_{0,2N-1})B_{2N-1} + (1 - \omega_{0,2N})B_{2N}), \\ \Delta \bar{B}_{2N}^s &= -\frac{1}{2} (\omega_{0,2N-1}T_{\text{scat},2N-1} + \omega_{0,2N}T_{\text{scat},2N}). \end{aligned}$$

4 Derivatives

4.1 Derivatives of Complex Mie Coefficients a_n and b_n

From Section 2.5 [8]

4.2 Mie Efficiency Temperature and Ice Water Content Derivatives

Mie efficiency temperature derivatives [8] are given by¹⁵

$$\begin{aligned}\frac{\partial \xi_s}{\partial T} &= \frac{4}{\chi^2} \sum_{n=1}^{n_{\text{cut}}} (2n+1) \left[\Re a_n \Re \frac{\partial a_n}{\partial T} + \Im a_n \Im \frac{\partial a_n}{\partial T} + \Re b_n \Re \frac{\partial b_n}{\partial T} + \Im b_n \Im \frac{\partial b_n}{\partial T} \right], \\ \frac{\partial \xi_e}{\partial T} &= \frac{2}{\chi^2} \sum_{n=1}^{n_{\text{cut}}} (2n+1) \left(\Re \frac{\partial a_n}{\partial T} + \Re \frac{\partial b_n}{\partial T} \right).\end{aligned}$$

Note that since ξ_s and ξ_e are not functions of Ice Water Content (IWC), we have

$$\begin{aligned}\frac{\partial \xi_s}{\partial I} &= 0, \\ \frac{\partial \xi_e}{\partial I} &= 0.\end{aligned}\tag{13}$$

4.3 Temperature and Ice Water Content Derivatives of β

The temperature derivatives of β_{c-e} and β_{c-s} [8] are:¹⁶ ¹⁷

$$\begin{aligned}\frac{\partial \beta_{c-e}}{\partial T} &= \pi \int_0^\infty r^2 \left(\frac{\partial n(r)}{\partial T} \xi_e(r) + n(r) \frac{\partial \xi_e(r)}{\partial T} \right) dr, \\ \frac{\partial \beta_{c-s}}{\partial T} &= \pi \int_0^\infty r^2 \left(\frac{\partial n(r)}{\partial T} \xi_s(r) + n(r) \frac{\partial \xi_s(r)}{\partial T} \right) dr.\end{aligned}$$

IWC derivatives of β_{c-e} and β_{c-s} [8] are:

$$\begin{aligned}\frac{\partial \beta_{c-e}}{\partial I} &= \pi \int_0^\infty r^2 \frac{\partial n(r)}{\partial I} \xi_e(r) dr, \\ \frac{\partial \beta_{c-s}}{\partial I} &= \pi \int_0^\infty r^2 \frac{\partial n(r)}{\partial I} \xi_s(r) dr.\end{aligned}$$

5 Additional materials

Tangent heights and angles for scattering calculations [13].

Organization of changes to Full Forward Model for TSCAT-computation mode [14].

Tasks for cloud forward model [15].

TScat and derivatives [16].

Current status of scattering additions to forward model [17].

Total IWC [18].

Accessing the TScat Jacobian as a Matrix T object [20].

Usage of Mie Tables program [21].

Full forward model changes to combine LBL, PFA and Tscat [24].

¹⁵Computed by Mie_Efficiencies.m, Mie_Efficiencies_Derivs function.

¹⁶Computed by Mie_Tables, function Do_dint_dBeta_dT.

¹⁷In Mie_Tables.f90, the descriptions are missing a factor π . However, calculations have a factor 2π .

6 Tscat Derivatives

- Path ray in full forward model
- → Incident rays used to precompute T_{scat}
- → Scattered rays from convolution of incident rays and phase function, i.e., T_{scat}
- + A_{mn} = Point at which atmospheric properties are provided during T_{scat} calculation
- ⊕ S_{jk} = Point at which T_{scat} is computed, i.e., incident rays are convolved with the phase function
- Point on the integration path
- Point on the integration path currently under consideration, properties interpolated from nearby S_{jk}

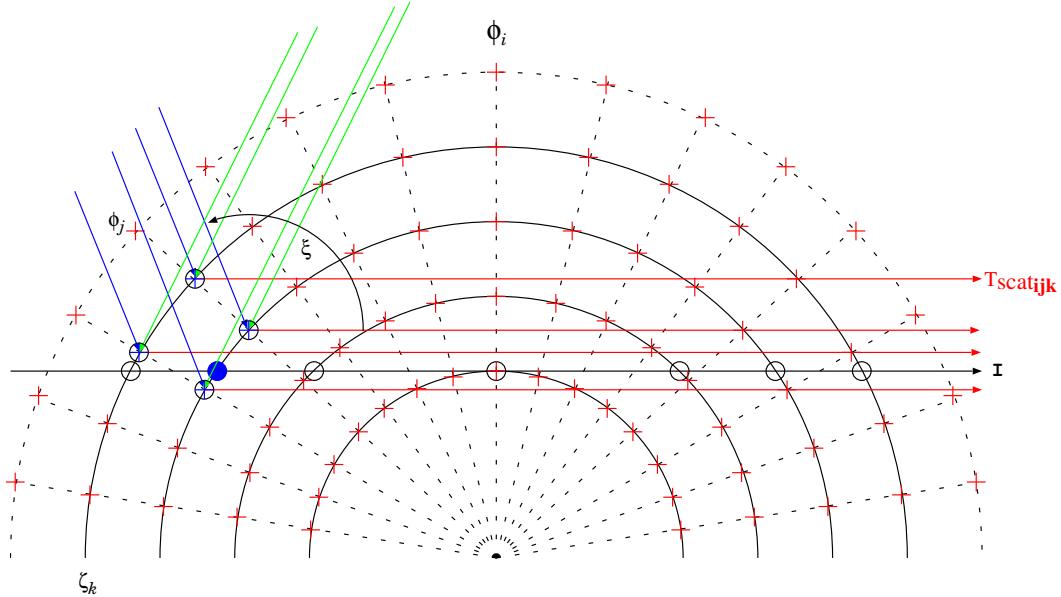


Figure 2: Tscat Geometry. This figure is taken from [19].

The reference orbit geodetic angle ϕ is denoted by ϕ_i .

The scattering points in the set $\{S_{jk}\}$, in the orbit plane, are on a grid specified by $\{\phi_j\} \times \{\zeta_k\}$, where $\{\phi_j\}$ are orbit geodetic angles and $\{\zeta_k\}$ are negative log pressures.

The reference horizon is the line in the orbit plane from the scattering point S_{jk} and perpendicular to the line in the orbit plane from the center of the Earth ϕ_i . [19], [26].

$P_{jk}(\xi)$ is the Mie scattering phase function, evaluated for ice water content and temperature at S_{jk} . $\xi = 0$ is at the reference horizon.

The radiance arriving at S_{jk} from direction ξ in the orbit plane is $I_{ijk}(\xi)$.

The radiance arriving at S_{jk} from all directions ξ in the orbit plane, convolved with the Mie phase function, is

$$T_{\text{scat}_{ijk}} = \bar{I}_{ijk} = \int_{-\pi}^{\pi} I_{ijk}(\xi) P_{jk}(\xi) d\xi.$$

The derivative of phase-convolved radiance at S_{jk} with respect to some quantity x_{mn} at A_{mn}

is

$$\frac{\partial \bar{I}_{ijk}}{\partial x_{mn}} = \begin{cases} \int_{-\pi}^{\pi} \frac{\partial I_{ijk}(\xi)}{\partial x_{mn}} P_{jk}(\xi) + I_{ijk}(\xi) \frac{\partial P_{jk}(\xi)}{\partial x_{mn}} d\xi, & \text{if } jk = mn, \\ \int_{-\pi}^{\pi} \frac{\partial I_{ijk}(\xi)}{\partial x_{mn}} P_{jk}(\xi) d\xi, & \text{if } jk \neq mn. \end{cases}$$

Remark: We can write $P_{jk}(\xi) = P(S_{jk}, \xi)$, $I_{ijk}(\xi) = I(\phi_i, S_{jk}, \xi)$, and $T_{\text{scat}_{ijk}} = T_{\text{scat}}(\phi_i, S_{jk})$.

7 Combining LBL and PFA

References: [4, 5, 23], [27] (Frequency Averaging).

The radiative transfer equation for line-by-line (LBL) calculations is

$$\begin{aligned} I_c &= \sum_{n=1}^{N_f} \phi_c(\nu_n) \Delta \nu_n I(\nu_n) \\ &= \sum_{n=1}^{N_f} \phi_c(\nu_n) \Delta \nu_n \sum_{i=1}^{N_p} \Delta B_i(\nu_n) \mathcal{T}_i(\nu_n), \\ I_c &= \sum_{n=1}^{N_f} \phi_c(\nu_n) \Delta \nu_n \sum_{i=1}^{N_p} \Delta B_i^g(\nu_n) \mathcal{T}_i(\nu_n) \\ &\quad + \sum_{i=1}^{N_p} \left(\hat{\mathcal{T}}_{i+1,c} T_{\text{scat}_{i+1,c}} - \hat{\mathcal{T}}_{i-1,c} T_{\text{scat}_{i-1,c}} \right) \\ \frac{\partial \omega_0}{\partial x} &= \frac{\partial}{\partial x} \left(\frac{\beta_{c,s}}{\beta_e} \right) = \frac{1}{\beta_e^2} \left(\beta_e \frac{\partial \beta_{c,s}}{\partial x} - \beta_{c,s} \frac{\partial \beta_e}{\partial x} \right) = \frac{1}{\beta_e^2} \left(\beta_e \frac{\partial \beta_{c,s}}{\partial x} - \beta_{c,s} \frac{\partial \beta_{c,e}}{\partial x} - \beta_{c,s} \frac{\partial \alpha_{\text{gas}}}{\partial x} \right) \\ &= \frac{1}{\beta_e} \left(\frac{\partial \beta_{c,s}}{\partial x} - \omega_0 \frac{\partial \beta_{c,e}}{\partial x} - \omega_0 \frac{\partial \alpha_{\text{gas}}}{\partial x} \right). \\ \frac{\partial I_c}{\partial x} &= \sum_{n=1}^{N_f} \phi_c(\nu_n) \Delta \nu_n \sum_{i=1}^{N_p} \left(\frac{\partial \Delta B_i^g(\nu_n)}{\partial x} \mathcal{T}_i(\nu_n) + \Delta B_i^g(\nu_n) \frac{\partial \mathcal{T}_i(\nu_n)}{\partial x} \right) \\ &\quad + \sum_{i=1}^{N_p} \left(\frac{\partial \hat{\mathcal{T}}_{i+1,c}}{\partial x} T_{\text{scat}_{i+1,c}} + \hat{\mathcal{T}}_{i+1,c} \frac{\partial T_{\text{scat}_{i+1,c}}}{\partial x} - \frac{\partial \hat{\mathcal{T}}_{i-1,c}}{\partial x} T_{\text{scat}_{i-1,c}} - \hat{\mathcal{T}}_{i-1,c} \frac{\partial T_{\text{scat}_{i-1,c}}}{\partial x} \right). \end{aligned}$$

8 Appendix: Spherical Bessel and Hankel Functions

$j_n(z)$ is the spherical Bessel function of first kind;

$y_n(z)$ is the spherical Bessel function of second kind;

$h_n^{(1)}(z)$ and $h_n^{(2)}(z)$ are the spherical Hankel function (or the spherical Bessel functions of the third kind).

8.1 Spherical Bessel Functions

When solving the Helmholtz equation in spherical coordinates by separation of variables, the radial equation has the form [25]:

$$z^2 \frac{d^2 w}{dz^2} + 2z \frac{dw}{dz} + (z^2 - n(n+1)) w = 0.$$

The solutions to this equation are called the spherical Bessel functions j_n and y_n , and are related to the ordinary Bessel functions J_n and Y_n by:

$$j_n(z) = \sqrt{\frac{\pi}{2z}} J_{n+\frac{1}{2}}(z) = (-1)^n \sqrt{\frac{\pi}{2z}} Y_{-n-\frac{1}{2}}(z),$$

$$y_n(z) = \sqrt{\frac{\pi}{2z}} Y_{n+\frac{1}{2}}(z) = (-1)^{n+1} \sqrt{\frac{\pi}{2z}} J_{-n-\frac{1}{2}}(z).$$

The spherical Bessel functions can also be written as:

$$j_n(z) = (-z)^n \left(\frac{1}{z} \frac{d}{dz} \right)^n \frac{\sin z}{z},$$

$$y_n(z) = -(-z)^n \left(\frac{1}{z} \frac{d}{dz} \right)^n \frac{\cos z}{z}.$$

The first few spherical Bessel functions are:

$$j_0(z) = \frac{\sin z}{z}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z}$$

$$j_2(z) = \left(\frac{3}{z^2} - 1 \right) \frac{\sin z}{z} - \frac{3 \cos z}{z^2},$$

and

$$y_0(z) = -\frac{\cos z}{z}$$

$$y_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z}$$

$$y_2(z) = \left(-\frac{3}{z^2} + 1 \right) \frac{\cos z}{z} - \frac{3 \sin z}{z^2}.$$

8.2 Spherical Hankel Functions

The spherical Hankel functions are:

$$h_n^{(1)}(x) = j_n(x) + iy_n(x),$$

$$h_n^{(2)}(x) = j_n(x) - iy_n(x).$$

A simple closed-form expression for the Bessel functions of half-integer order in terms of the standard trigonometric functions, and therefore for the spherical Bessel functions, for non-negative integers n is:

$$h_n^{(1)}(x) = (-i)^{n+1} \frac{e^{ix}}{x} \sum_{m=0}^n \frac{i^m}{m!(2x)^m} \frac{(n+m)!}{(n-m)!}$$

and $h_n^{(2)}$ is the complex-conjugate of this (for real x). From this, it follows that

$$h_0^{(1)}(x) = \frac{\sin x}{x} - i \frac{\cos x}{x}$$

$$h_0^{(2)}(x) = \frac{\sin x}{x} + i \frac{\cos x}{x}$$

$$h_1^{(1)}(x) = -\frac{\cos x}{x} + \frac{\sin x}{x^2} + i \left(-\frac{\sin x}{x} - \frac{\cos x}{x^2} \right)$$

$$h_1^{(2)}(x) = -\frac{\cos x}{x} + \frac{\sin x}{x^2} - i \left(-\frac{\sin x}{x} - \frac{\cos x}{x^2} \right)$$

In other words, Hankel functions have always division by x to some power. This is what is done in sphbes.f90. However, it does not agree with initial conditions as in wvs-058 and ATBD.

8.3 Recurrence Relations and Derivatives

If $f_n(z)$ is $j_n(z), y_n(z), h_n^{(1)}(z), h_n^{(2)}(z)$, then

$$f_{n-1}(z) + f_{n+1}(z) = \left(\frac{2n+1}{z} \right) f_n(z).$$

Substituting $n+1 \rightarrow n$, this can be re-written as

$$f_{n-2}(z) + f_n(z) = \left(\frac{2n-1}{z} \right) f_{n-1}(z).$$

Using these expressions, we can find:

$$j_{-1}(z) = \frac{\cos z}{z}$$

$$y_{-1}(z) = \frac{\sin z}{z}$$

Bessel functions [1, 3, 25, 6]

8.4 Derivation of an equality

We consider equations from DLMF (equation numbering is from dlmf site):

$$\frac{\partial j_n(x)}{\partial x} = \frac{n}{x} j_n(x) - j_{n+1}(x) \quad (10.51.2)$$

$$j_{n+1}(x) = \frac{2n+1}{x} j_n(x) - j_{n-1}(x) \quad (10.51.1)$$

Plugging (10.51.1) into (10.51.2):

$$\frac{\partial j_n(x)}{\partial x} = \frac{n}{x} j_n(x) - \left(\frac{2n+1}{x} j_n(x) - j_{n-1}(x) \right) = j_{n-1}(x) - \frac{n+1}{x} j_n(x).$$

We plug this into the right hand side of (??):

$$\begin{aligned} \frac{1}{2x} + \frac{1}{j_n(x)} \frac{\partial j_n(x)}{\partial x} &= \frac{1}{2x} + \frac{1}{j_n(x)} \left(j_{n-1}(x) - \frac{n+1}{x} j_n(x) \right) \\ &= \frac{1}{2x} - \frac{n+1}{x} + \frac{j_{n-1}(x)}{j_n(x)} \\ &= -\frac{2n+1}{2x} + \frac{j_{n-1}(x)}{j_n(x)} \\ &= -\frac{1}{2x} - \frac{n}{x} + \frac{j_{n-1}(x)}{j_n(x)}. \end{aligned}$$

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