

Application of exponential series to calculation of radiative fluxes in the molecular atmosphere

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Received July 8, 1999

Exponential series as an approach to radiation intensity integration over spectrum are most efficient in solution of the problems associated with radiative processes in the atmosphere as applied to derivation of equations for spectrally mean parameters.

1. Statement of the problem

Let us use the designation $J(\mathbf{r}, \mathbf{n}; \omega)$ for the spectral (at the frequency ω) intensity of radiation coming through the point \mathbf{r} in the direction of the unit vector \mathbf{n} . The parameter

$$\mathbf{F}(\mathbf{r}) = \int \mathbf{n} J(\mathbf{r}, \mathbf{n}; \omega) d\mathbf{n} d\omega \quad (1)$$

is called the radiative flux at the point \mathbf{r} , and

$$\operatorname{div} \mathbf{F} = 4\pi \int d\omega \eta(\mathbf{r}, \omega) - \int d\omega d\mathbf{n} \kappa(\mathbf{r}, \omega) J(\mathbf{r}, \mathbf{n}; \omega) \quad (2)$$

enters into the equation of heat balance at the point \mathbf{r} (more exactly, the corresponding elementary volume); the values η and κ in Eq. (2) are the coefficients of emission and absorption. Of course, the situation is assumed stationary in the sense that there are no processes in the medium whose speed is comparable with the speed of light, and therefore the time t enters into the transfer equation only as a parameter. Then (keeping in mind, as usually, that the transfer equation deals with the rays of geometrical optics) $\mathbf{n}J$ is interpreted as the Poynting vector, and Eq. (2) proves to be the Joule heat.

We consider the popular situation for radiative problems^{1,2}: the horizontally inhomogeneous plane molecular atmosphere in which the transfer equation has the following form:

$$\cos \theta \frac{\partial J(z, \theta; \omega)}{\partial z} = -\kappa(z, \omega) J(z, \theta; \omega) + \eta(z, \omega). \quad (3)$$

Here z is the altitude above the Earth's surface; θ is the angle between the vertical and the direction of ray propagation. Recall that $\eta = B\kappa$ with the Planck function $B(\omega, \Theta)$ in the case of local thermodynamic equilibrium (LTE) at the temperature Θ . Sometimes (high atmospheric layers,³ far wing of a water vapor rotational band⁴) b should be multiplied by the factor $\mu(\omega)$ responsible for deviation from LTE.

The main computational problem is connected with the need, because of Eqs. (1) and (2), to integrate the solution (3) over frequency. Modern computers and the line-by-line procedure seemingly

allow us to treat this problem as purely technical. However, some new, rather significant circumstances arise. The principal point is that the quantum calculation of $\kappa(\omega)$ is accompanied by numerous approximations and the need to involve a huge number of empirical constants. At the same time, for Eq. (1) there is no need in thus detailed spectroscopic pattern, so we have to remove the "excess" information (which is obtained in a rather intricate way) by applying an additional, also rather intricate, effort. Moreover, an abundance of spectral lines makes the radiative block of climate models and algorithms of geophysical applications of atmospheric optics so cumbersome that sometimes efficient functioning of such models and algorithms is quite questionable. That is why the approaches of the pre-computer era again become popular; this is a sort of Renascence of ideas for calculation of $\int d\omega (\dots)$ in Eq. (1).

One of the ideas is in application of exponential series, which leads for Eq. (3) (see Ref. 5) to the equations

$$I(z, \theta) \equiv \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} J(z, \theta; \omega) d\omega = \sum_{\nu=1} b_{\nu} I_{\nu}(z, \theta), \quad (4)$$

$$\Delta\omega = \omega'' - \omega';$$

$$\cos \theta \frac{\partial I_{\nu}(z, \theta)}{\partial z} = -s(g_{\nu}; z) I_{\nu} + \Omega(z) s(g_{\nu}; z). \quad (5)$$

Here b_{ν} and g_{ν} are the ordinates and abscissas of the quadrature formula; $s(g, z)$ is the function inverse to $g(s; z)$ (by the argument s ; z is treated as a parameter):

$$g(s; z) = \frac{1}{\Delta\omega} \int_{\kappa(\omega; z) \leq s, \omega \in [\omega', \omega'']} u(\omega; z) d\omega;$$

$$u(\omega; z) = \frac{B(z, \omega)}{\Omega(z)};$$

$$\Omega(z) = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} d\omega B(z, \omega).$$

In the case of LTE violation, B in Eq. (6) should be replaced by B_{μ} ; the dependence of b on z is caused by $\Theta = \Theta(z)$.

Equation (4) shows that Eq. (5) is the equation for intensity already integrated over frequency. The procedure of transition from Eq. (3) to Eq. (5) is practically exact. Then let us follow up the sequential application of Eqs. (4) and (5) to calculation of Eq. (2).

Here there are two points to be noted as applied to the program appealing to Eqs. (4)–(6). First, the procedure (6) of constructing $s(g)$, as found, is reduced to a certain ordering of $\kappa(\omega)$ by value. Second, with the proper choice of the quadrature function, the Eq. (4) includes only several terms in spite of thousands terms as in the case of direct integration $\int d\omega (\dots)$ in Eq. (4).

In this context, let us also remind that Eq. (2) enters into the thermodynamic relation^{1,2}

$$c_p \rho \frac{\partial \Theta}{\partial t} = -\text{div } \mathbf{F} + G \quad (7)$$

for the temperature variation at a certain point. Here ρ is the air density; c_p is the heat capacity at constant pressure; the term G includes other factors, different from the radiative flux, that change the temperature (for example, convection). As was already mentioned, it is just Eq. (7) that causes the parametric time dependence in Eq. (5).

2. Solution

The integral of Eq. (5) is

$$I_{\nu}(z, \theta) = \sec \theta C e^{-\sec \theta \int_{z_0}^z s(g_{\nu}; z') dz'} + \sec \theta \int_{z_0}^z dz' \Omega(z') s(g_{\nu}; z') e^{-\sec \theta \int_{z'}^z s(g_{\nu}; z'') dz''} \quad (8)$$

with the integration constants C and z_0 . The first term in Eq. (8) is the solution of the homogeneous equation corresponding to Eq. (5), while the second term is the solution of the inhomogeneous equation.

The latter has the meaning of atmospheric emission or diffuse radiation. To calculate it, we should formally assume $C = 0$. Usually, the diffuse radiation is separated into downward I^{\downarrow} ($z_0 = \infty$; $\pi/2 < \theta < \pi$), and upward I^{\uparrow} ($z_0 = 0$; $0 \leq \theta < \pi/2$) going components with $I_{\nu}(z, \pi/2) = 0$, what immediately follows from Eq. (8). So,

$$I_{\nu}^{\downarrow} = -\sec \theta \int_z^{\infty} dz' \Omega(z') s(g_{\nu}; z) e^{\sec \theta \int_z^{z'} s(g_{\nu}; z'') dz''} \quad ; \quad (9)$$

$$I_{\nu}^{\uparrow} = \sec \theta \int_0^z dz' \Omega(z') s(g_{\nu}; z) e^{-\sec \theta \int_{z'}^z s(g_{\nu}; z'') dz''} \quad . \quad (10)$$

For the downward going radiation, the solar radiation naturally plays the part of the solution to the homogeneous equation; it formally bounds the constant C . To avoid some mathematical troubles, we may simply return to Eqs. (1) and (3): if the unit vector \mathbf{n}_0 determines the direction of solar rays and $J^{(0)}(\omega)$ describes their spectral composition, then Eq. (9) should be supplemented with

$$I_{\nu}^{(0)} = K \delta(\mathbf{n} - \mathbf{n}_0) e^{\sec \theta \int_z^{\infty} p(g_{\nu}; z') dz'} \quad (11)$$

Again we consider the procedure (6) with the replacements

$$u \rightarrow v = \frac{J^{(0)}(\omega)}{K}, \quad \Omega \rightarrow K = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} J^{(0)}(\omega) d\omega, \quad s \rightarrow p.$$

The Earth's radiation is taken into account just similarly in calculation of the upward going radiation. It is usually assumed isotropic over θ and having some spectral composition $J_0(\omega)$. Equation (10) is supplemented with

$$I_{0\nu} = N e^{-\sec \theta \int_0^z q(g_{\nu}; z') dz'} \quad (12)$$

and in the procedure (6)

$$u \rightarrow n(\omega) = \frac{J_0(\omega)}{N}, \quad N = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} J_0(\omega) d\omega, \quad s \rightarrow q.$$

One more term in the upward going radiation follows from reflection of the downward going radiation from the underlying surface. As known, this problem is discussed rather differently than the similar problem in electrodynamics. The macroscopic underlying surface with its obvious "roughness" and other factors drastically "processing" the radiation incident on it reflects as a Lambertian surface and responds to the total (integral over ω) radiative flux (i.e. by the value of the type (1)). From this we have the definition of the spectral albedo

$$A(\omega) = \frac{\text{reflected spectral flux}}{\text{total incident flux } F^{\downarrow}(z=0)}.$$

Therefore, the spectral intensity of reflected radiation is

$$\frac{A(\omega)}{\pi} F^{\downarrow}(z=0) = \tilde{J}_0(\omega)$$

(π is the normalization factor corresponding to the definition of A). The rest remains the same as in Eq. (12), and so we have

$$I_{0\nu} = N' e^{-\sec \theta \int_0^z q'(g_{\nu}; z') dz'} \quad (13)$$

with the replacements

$$n \rightarrow n'(\omega) = \frac{A(\omega)}{\frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} A(\omega) d\omega},$$

$$N \rightarrow N' = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} \tilde{J}_0(\omega) d\omega, \quad q \rightarrow q'.$$

Thus, the intensity of the downward going radiation is

$$I^\downarrow = \sum_{v=1} b_v [(9) + (11)], \quad \frac{\pi}{2} < \theta \leq \pi \quad (14)$$

while the intensity of the upward going radiation is

$$I^\uparrow = \sum_{v=1} b_v [(10) + (12) + (13)]. \quad (15)$$

Arguments in Eqs. (14) and (15) are only z and θ , so, by the definition (7),

$$\begin{aligned} \operatorname{div} \mathbf{F} &= \frac{\partial F_3}{\partial z} \equiv \frac{\partial F}{\partial z}, \\ F &= 2\pi \left\{ \int_0^{\pi/2} \{(15)\} \sin \theta \cos \theta d\theta - \int_{\pi/2}^{\pi} \{(14)\} \sin \theta \cos \theta d\theta \right\} \equiv \\ &\equiv F^\uparrow - F^\downarrow. \end{aligned} \quad (16)$$

The minus sign appears because the third axis of the coordinate system (F_3 , the corresponding component of \mathbf{F}) is directed along the vertical. The integrals over θ in Eq. (16) can easily be reduced to the integral exponential function

$$E_m(y) = \int_1^\infty \frac{e^{-y\xi} d\xi}{\xi^m}, \quad m = 0, 1, 2, \dots,$$

and here it is obvious significance that the simple exponential structure of the solution (8) survives.

The next stage is connected with the transition to the model of stratified atmosphere: the atmosphere is assumed consisting of layers (k is the index of a layer; z_{k-1} and z_k are its boundaries, $l_k = z_k - z_{k-1}$ is the layer thickness; $k = 1, 2, \dots$, starting from the ground), and thermodynamic characteristics (temperature, pressure, concentration of absorbing gases) are assumed constant within a layer. (The layer's index k is assigned to them either, for example, Θ_k and ρ_k in Eq. (7)). The aim of this action is to pass from Eq. (7) with partial derivatives to the system of ordinary differential equations for Θ_k .

Such a model assumes a possibility of neglecting the microstructure of a layer (it may prove significant, for example, when considering convection), and Eq. (7) can formally be averaged by the operation

$$(1/l_k) \int_{z_{k-1}}^{z_k} dz \text{ which gives rise to the term } c_p \rho_k \partial \Theta_k / \partial t$$

in the left-hand side of the equation. In the right-hand side of the equation, direct integration (16):

$$\frac{1}{l_k} \int_{z_{k-1}}^{z_k} \left(-\frac{\partial F}{\partial z} \right) dz = \frac{1}{l_k} [F(z_{k-1}) - F(z_k)], \quad (17)$$

is possible, because F is already considered as depending on average macroscopic characteristics of the layer, and Eq. (7) is actually transformed into the system of equations for them. Equation (17) reduces the problem to calculation of fluxes at a certain level – the layer's boundary.

The algorithm for calculation of $F(z_k)$ is simple, and we illustrate it using as an example of the downward going diffuse flux: Eq. (8) is substituted in Eq. (16) successively for $z = z_1, z_2, \dots$. In the following formulas Ω_k and $s_k(g_k)$ are Ω in the k th layer and $\tau_k^{(v)} = s_k(g_v) l_k$.

The result is obvious at $z \rightarrow z_1$:

$$\begin{aligned} I_v^\uparrow(z_1) &= \sec \theta \int_{z_0}^{z_1} dz' \Omega(z') s(g_v; z') e^{-\sec \theta \int_{z'}^z s(g_v; z'') dz''} = \\ &= \Omega_1 s_1(g_v) \int_{z_0}^{z_1} dz' e^{-s_1(g_v) \sec \theta (z_1 - z')}. \end{aligned}$$

If $z \rightarrow z_2$, then $\int_{z_0}^{z_2} dz' = \int_{z_0}^{z_1} dz' + \int_{z_1}^{z_2} dz'$ with its own

Ω_k and s_k for each term:

$$\begin{aligned} I_v^\uparrow(z_2) &= \Omega_1 s_1 \sec \theta \int_{z_0}^{z_1} dz' e^{-\sec \theta \{s_1(z_1 - z') + s_2 l_2\}} + \\ &+ \Omega_2 s_2 \sec \theta \int_{z_1}^{z_2} dz' e^{-s_2 \sec \theta (z_2 - z')}. \end{aligned}$$

By the same procedure we obtain that

$$\begin{aligned} I_v^\uparrow(z_3) &= \Omega_1 s_1 \sec \theta \int_{z_0}^{z_1} dz' e^{-\sec \theta \{s_1(z_1 - z') + s_2 l_2 + s_3 l_3\}} + \\ &+ \Omega_2 s_2 \sec \theta \int_{z_1}^{z_2} dz' e^{-\sec \theta \{s_2(z_2 - z') + s_3 l_3\}} + \\ &+ \Omega_3 s_3 \sec \theta \int_{z_2}^{z_3} dz' e^{-\sec \theta s_3(z_3 - z')} \end{aligned}$$

and so on. Upon the following integration over z' and θ we have

$$\begin{aligned} F_v^\uparrow(z_1) &= \pi \Omega_1 - 2\pi E_3(\tau_1^{(v)}), \\ &\dots\dots \\ F_v^\uparrow(z_k) &= \pi \Omega_k - 2\pi (\Omega_k - \Omega_{k-1}) E_3(\tau_k^{(v)}) - \\ &- 2\pi (\Omega_{k-1} - \Omega_{k-2}) E_3(\tau_k^{(v)} + \tau_{k-1}^{(v)}) - \\ &- 2\pi (\Omega_{k-2} - \Omega_{k-3}) E_3(\tau_k^{(v)} + \tau_{k-1}^{(v)} + \tau_{k-2}^{(v)}) - \dots - \\ &- 2\pi (\Omega_2 - \Omega_1) E_3(\tau_k^{(v)} + \tau_{k-1}^{(v)} + \dots + \tau_2^{(v)}) - \\ &- 2\pi \Omega_1 E_3(\tau_k^{(v)} + \tau_{k-1}^{(v)} + \dots + \tau_1^{(v)}). \end{aligned} \quad (18)$$

The downward going diffuse flux is calculated in perfect analogy (the subscript j is for the upper layer; the minus sign is already taken into account) as:

$$F_v^\downarrow(z_{j-1}) = -\pi \Omega_j + 2\pi E_3(\tau_j^{(v)}),$$

$$F_v^\downarrow(z_{j-k}) = -\pi \Omega_{j-k+1} + 2\pi(\Omega_{j-k+1} - \Omega_{j-k+2})E_3(\tau_{j-k+1}^{(v)}) +$$

$$+ 2\pi(\Omega_{j-k+2} - \Omega_{j-k+3})E_3(\tau_{j-k+1}^{(v)} + \tau_{j-k+2}^{(v)}) + \dots +$$

$$+ 2\pi(\Omega_{j-1} - \Omega_j)E_3(\tau_{j-k+1}^{(v)} + \tau_{j-k+2}^{(v)} + \dots + \tau_{j-1}^{(v)}) +$$

$$+ 2\pi \Omega_j E_3(\tau_{j-k+1}^{(v)} + \tau_{j-k+2}^{(v)} + \dots + \tau_j^{(v)}).$$

The case of solar fluxes is rather easy: the constant K from Eq. (11) is multiplied by $\cos \theta_0$ (θ_0 is the direction of the solar rays) and for the layer z_{j-k} by

$$\exp(-\tilde{\tau}_{j-k+1}^{(v)} - \tilde{\tau}_{j-k+2}^{(v)} - \dots - \tilde{\tau}_j^{(v)})$$

with $\tilde{\tau}_k^{(v)} = l_k p_k(g_v)$. The fluxes from the underlying surface are the constants N and N' from Eqs. (12) and (13) multiplied by $2\pi E_3$ whose arguments for the level z_k are $e_1 q_1(g_v) + e_2 q_2(g_v) + \dots + e_k q_k(g_v)$ or $e_1 q_1'(g_v) + e_2 q_2'(g_v) + \dots + e_k q_k'(g_v)$.

3. Subsequent approximations

Many computational techniques (see, for example, Ref. 6) try to present the fluxes in terms of the transmission function

$$Q = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} e^{-x\kappa(\omega)} d\omega$$

for the path of the beam of length x in a homogeneous medium. Medium inhomogeneity is then taken into account by using "average" pressure and temperature,^{3,7} whereas the diffuse character of radiation (integration (16)) is taken into account by multiplying the optical density $\tau = x\kappa$ by a properly chosen factor.³ The practical significance of this action is obvious: it allows one to use the experimental (or other) information directly for the absorption function $1 - Q$.

The application of exponential series for Q yields the series⁸:

$$Q = \sum_v b_v e^{-x s(g_v)}, \tag{19}$$

where $s(g)$ is the function inverse to

$$g(s) = \frac{1}{\Delta\omega} \int_{\kappa(\omega) \leq s, \omega \in [\omega', \omega'']} d\omega.$$

Comparing this equation with Eq. (16), we see that the condition of passing to the discussed version is $u \cong 1$; the same is true for v, n , and n' written after Eqs. (11), (12), and (13).

Even more simple scheme (see, for example, Ref. 9) appears for the heuristic, in its essence, expression written for the flux (for example, upward going one)

$$F(z_k) - F(z_{k-1}) = -(1 - Q)F(z_{k-1}) + D_k(1 - Q) \tag{20}$$

with the obvious meaning of the terms. The symbol D_k is used for the total radiative flux of the black body at Θ_k . In our designations $D_k = \pi \Theta_k$, if $\int d\omega$ is assumed to be performed over the entire spectrum.

Of course, Eq. (20) can be simply treated as a definition of some parameter

$$1 - Q = \frac{F(z_k) - F(z_{k-1})}{\pi \Omega_k - F(z_{k-1})}, \tag{21}$$

and what we need is only to see when Q actually becomes the transmission function of the layer under consideration. Let us consider this problem from the position presented by Eqs. (18), assuming of course that Eq. (21) deals with F_v^\uparrow . To be certain, we assume $k = 4$; at the same time, this version is completely representative for explanation of the approximation.

Thus, under our assumptions, the numerator and denominator of Eq. (21) are

$$\pi(\Omega_4 - \Omega_3)[1 - 2E_3(\tau_4^{(v)})] +$$

$$+ 2\pi(\Omega_3 - \Omega_2)[E_3(\tau_3^{(v)}) - E_3(\tau_3^{(v)} + \tau_4^{(v)})] +$$

$$+ 2\pi(\Omega_2 - \Omega_1)[E_3(\tau_2^{(v)} + \tau_3^{(v)}) - E_3(\tau_2^{(v)} + \tau_3^{(v)} + \tau_4^{(v)})] +$$

$$+ 2\pi\Omega_1[E_3(\tau_1^{(v)} + \tau_2^{(v)} + \tau_3^{(v)}) - E_3(\tau_1^{(v)} + \tau_2^{(v)} + \tau_3^{(v)} + \tau_4^{(v)})];$$

$$\pi(\Omega_4 - \Omega_3) + 2\pi(\Omega_3 - \Omega_2)E_3(\tau_3^{(v)}) +$$

$$+ 2\pi(\Omega_2 - \Omega_1)E_3(\tau_2^{(v)} + \tau_3^{(v)}) + 2\pi\Omega_1 E_3(\tau_1^{(v)} + \tau_2^{(v)} + \tau_3^{(v)}).$$

Then, as follows from the definition of E_m ,

$$E_3(a) - E_3(a + b) = E_3(a) \left(1 - \frac{E_3(a + b)}{E_3(a)} \right) =$$

$$= E_3(a) \left\{ \frac{E_2(a)}{E_3(a)} b - \frac{E_1(a)}{E_3(a)} \frac{1}{2!} b^2 + \frac{E_0(a)}{E_3(a)} \frac{1}{3!} b^3 + \dots \right\},$$

if $b \ll a$. Besides, if we take $a \gg 1$, then $E_m'/E_m \rightarrow 1$ and under our assumptions the expression in the braces can be replaced by $[1 - \exp(-b)]$. The same expression is asymptotic for $[1 - 2E_3(b)]$ also at $b \gg 1$.

In our case the role of b is played by $\tau_k^{(v)}$ (optical density of the chosen layer). It should be assumed small as compared with the sum of optical densities of "preceding" layers which is sufficiently large. At the same time, $\tau_k^{(v)}$ itself must be not very large. Under such conditions, the ratio of the numerator and denominator is $[1 - \exp(-\tau_k^{(v)})]$, what essentially coincides with Q in Eq. (20) with the account of Eq. (19).

It is sometimes more convenient to use equations of the type (18) in the form including the derivatives of $\Omega(z)$, because they vanish for the isothermal atmosphere, what certainly simplifies analysis of some physical situations, for example, those close to isothermal. Here we should first perform integration in Eq. (16) after substitution of the corresponding integrands, transform $\int dz'$ by integration by parts, and use known properties of E_m during the transition to the stratified atmosphere. Thus, for example, we have the following expression, instead of Eq. (18),

$$\begin{aligned} I_{\nu}^{\uparrow}(z_k) = & \pi\Omega(z_k) - 2\pi \frac{\Omega_1'}{s_1(g_{\nu})} \times \\ & \times [E_4(\tau_k^{(\nu)} + \dots + \tau_2^{(\nu)}) - E_4(\tau_k^{(\nu)} + \tau_{k-1}^{(\nu)} + \dots + \tau_1^{(\nu)})] + \\ & + \frac{\Omega_2'}{s_2(g_{\nu})} [E_4(\tau_k^{(\nu)} + \dots + \tau_3^{(\nu)}) - E_4(\tau_k^{(\nu)} + \tau_{k-1}^{(\nu)} + \dots + \\ & + \tau_2^{(\nu)})] + \dots + \frac{\Omega_{k-1}'}{s_{k-1}(g_{\nu})} [E_4(\tau_k^{(\nu)} - E_4(\tau_k^{(\nu)} + \tau_{k-1}^{(\nu)})] + \\ & + \frac{\Omega_k'}{s_k(g_{\nu})} [E_4(0) - E_4(\tau_k^{(\nu)})]. \end{aligned}$$

Here Ω_k' is $d\Omega(z)/dz$ for the k th layer.

Acknowledgments

This work was partially supported by the Russian Foundation for Basic Research, Grant No. 97-05-65985.

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