USE OF DIRICHLET SERIES IN ATMOSPHERIC OPTICS

S.D. Tvorogov

Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk
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In this paper I'd like to discuss some problems arising when applying Dirichlet series to calculations of spectrally integrated radiation characteristics and give a review of the results obtained at the Institute of Atmospheric Optics SB of RAS, which give answers to many methodical and computational questions.

1. INTRODUCTION INTO THE PROBLEM ON USING THE SERIES OF EXPONENTS AS A METHOD FOR ANALYZING THE ABSORPTION FUNCTIONS

The specific features of the atmospheric spectroscopy are a great extent caused by the necessity of related calculating the absorption function Q of atmospheric gases.[1,2] First of all, it is the integration over frequency ω of the "palisade" of a great number of spectral lines. The overlapping of the absorption bands of different gases makes additional troubles in calculations since the total absorption function Q is by no means a product of the absorption functions of the gaseous constituents, while they are just the values, which are measured experimentally. It is impossible to write Q for an inhomogeneous (relative to thermodynamic parameters) medium even if Q is available for any thermodynamically homogeneous case. Finally, it is often necessary to know the "source function", i.e. a solution of the problem on light propagation in absorbing and emitting molecular atmosphere integrated over the spectrum.

These problems become much more complicated in climate models because the program for calculating Q should be only a small part of the entire computer model. However, requirements to the calculation accuracy remain very high.

Convincing illustration to the subject of the discussion is the radiation transfer equation for a aerosol-molecular medium. The molecular absorption, which is trivial in the problem of wave propagation arises all the above questions when calculating the values integrated over the spectrum. At the same time light scattering, which produces the main mathematical difficulties is independent of ω in a wide spectral interval. The situation seems to be very poor, since we shall have to iteratively solve the transfer equation changing in each iteration only the molecular absorption coefficient entering it as a parameter and then, in addition, to integrate over ω numerically.

One of the popular approaches to resolve these problems is the use of series of exponents. The original idea was proposed by V.A. Ambartsumyan in 1936 as early, and now there are some reviews, see, for example, Refs. 3—19 and the references therein.

Let us illustrate the mathematical definitions using the transmission function, (which is equal $1 - Q$), as an example

$$F(x) = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} d\omega \, \exp\left(-x \, \kappa(\omega)\right) \qquad (1)$$

for the ray path length x in a homogeneous medium with the molecular absorption coefficient $\kappa(\omega)$ in the spectral interval $\Delta\omega = \omega'' - \omega'$. A series of exponents that is used as a representation of Eq. (1) has the form

$$F(x) = \sum_{\nu} b_{\nu} \exp\left(-s_{\nu} x\right) \quad (2)$$

with the abscissas s_{ν} and ordinates b_{ν}.

The case with the transfer equation clearly explains the pragmatic importance of Eq. (2). As it follows from Ref. 20, now the integral intensity is $\sum_{\nu} b_{\nu} I_{\nu}$, where I_{ν} is the solution of the transfer equation, in which the "ordinary numbers" s_{ν} replace $\kappa(\omega)$. In so doing the transfer equation should be solved as many times as is the number of terms in the sum (2).

It is obvious, that the efficiency of Eq. (2) is entirely regulated by a proper choice of b_{ν} and s_{ν} quantities. Let us briefly discuss some aspects essential to the history of the problem.

The idea (2) has long been associated with the Laplace transform

$$F(x) = \int_{0}^{\infty} ds \, f(s) \, \exp\left(-sx\right) , \qquad (3)$$

since, the change of the integral for an appropriate quadrature formula for $f(s)$ would suit quite well. For example, of a Gaussian type, would minimize the number of terms in Eq. (2). The function $f(s)$ is often taken as corresponding to $F(x)$ for certain models of the absorption bands with a corrections to their parameters made in accordance with the experimental or calculated data using the theoretical $\kappa(\omega)$. Of course, one can find much grounds for criticizing such an approach. However, there is no denying that this way exhibits quite good pragmatic rationality.

The idea seems to be very attractive to treat b_ν as the probability density ($\sum_\nu b_\nu = 1$ follows from Eqs. (1) and (2) at $x = 0$) of $\kappa(\omega)$ being equal to s_ν. In this case one may use (say, when considering the overlapping spectra) the formal rules of the probability theory. As a result it seems so that Eq. (3) may make a ground for such a position. Actually, it follows from Eqs. (2) and (5) that

$$f(s) = \frac{1}{2\pi i} \int_{c - i\infty}^{c + i\infty} dx \, \exp(sx) \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} d\omega \, \exp(-x\,\kappa(\omega)) ,$$

$$c > 0 . \tag{4}$$

If to interchange the integrations in Eq. (4) the function $f(s) = (\Delta\omega)^{-1} \int_{\omega'}^{\omega''} \delta(s - \kappa(\omega)) d\omega$ appears. The δ − function, which appears here, leads to the distribution function for the value s according to the known scenarium of the probability theory. However by making use of the standard procedures of the mathematical analysis it is simple to establish that the interchange of the integrations in Eq. (4) is impossible and therefore the probabilistic interpretation of the ordinates in Eq. (2) remains only an arbitrary statement.

The importance of the mathematical element (4) under discussion is even more wide. Actually, the last (and incorrect) version results in $f = \sum (\Delta\omega)^{-1} |\kappa'(\tilde\omega(s))|^{-1}$ with the sum over the roots $\tilde\omega$ (s) of the equation $\kappa(\omega) = s$. In fact, this same expression appears after the substitution of the integration variable $s = \kappa(\omega)$ in Eq. (1). However, this action is forbidden because the extreme points, where $\kappa'(\omega) = 0$, are inevitable by the very structure of $\kappa(\omega)$ which is a sum of spectral lines. It is for this reason, the roundabout way of constructing $f(s)$ appears to be necessary.

There is no doubts that a procedure is needed for Eq. (2), which first, allows the values b_ν and s_ν to be calculated immediately in terms of $\kappa(\omega)$, and, second, it should be invariant relative to all the above mentioned problems with the absorption function.

Furthermore, in many papers devoted to Eq. (2) the "physical level of rigor" prevails though the present-day theory of the Dirichlet series[21—23] (that is how mathematicians call the expansions like Eq. (2)) provides for a much more sophisticated "mathematical climate." (As an example, the popular relationship between f and $\kappa'(\omega)$ should be mentioned, which is a consequence of mathematically incorrect use of Eq. (4)).

We consider the latter circumstances as an evidence of the fact that the potential capabilities of the method "series of exponents" are not yet properly realized and the papers[24—29] can be considered as an illustration of this statement. The discussion of such new elements makes the subject of this paper.

2. THE METHOD OF CALCULATING THE COEFFICIENTS OF A SERIES OF EXPONENTS USING SPECTROSCOPIC DATABASES.

The main idea of the method proposed can be most simply explained when considering the case of a homogeneous medium assuming Eq. (1) to be the initial value.

First, the mathematical problem arising in Eq. (4) should be overcome to save the very constructive idea of the relation between Eqs. (2) and (3). This happens to be achieved by introducing the function

$$g(s) = \int_0^s f(s) \, ds = \frac{1}{2\pi i} \int_{c - i\infty}^{c + i\infty} \frac{dx}{x} F(x) \exp(sx) . \tag{5}$$

It is evident that Eqs.(3)—(5) lead to

$$F(x) = \int_0^1 dg \, \exp(-xs(g)) , \quad s(g) \equiv g^{-1}(g) . \tag{6}$$

When F in Eq.(5) is replaced by Eq. (1) the interchange of integrations is already possible and that allows the basic formula of the method to be derived

$$g(s) = \frac{1}{\Delta\omega} \int_{\kappa(\omega) \le s; \, \omega \in [\omega',\omega'']} d\omega . \tag{7}$$

The transition from Eq. (6) to Eq. (2) is made simply by applying the quadrature formulas

$$F(x) = \sum_\nu b_\nu \exp(-xs(g_\nu)). \tag{8}$$

As numerical estimates show it is sufficient to take no more than 5 or 6 terms in the series (8) when using the formulas of the Gauss or Chebyshev type (g_ν are their abscissas).

It is essential that b_ν in Eq. (8) are simply the numbers, i.e. the ordinates of formulas for numerical integration and the dependence on thermodynamical parameters of the medium is entirely presented by $s(g)$. This circumstance is very significant when solving the above problems of atmospheric spectroscopy and this makes Eq. (8) favorably different than the equation following from Eq. (3)

$$F(x) = \sum_\nu a_\nu \exp(-x s_\nu) . \qquad (9)$$

In Eq. (9) the abscissas s are simply the numbers as well, however, the physical values enter the ordinates g_ν.

It seems to be interesting to consider some fine details of a comparison between Eqs. (8) and (9) are of some interest. It follows from the theory of the Dirichlet series that in Eq. (9)

$$s_\nu = \lambda_\nu , \qquad a_\nu = \int_0^\infty \frac{L(s) f(s) \, ds}{\lambda - \lambda_\nu} \frac{1}{L'(\lambda_\nu)} .$$

The integral function $L(\lambda)$ with simple roots λ_ν should appear in the expansion of the exponent

$$\exp(-\lambda x) = \sum_\nu \frac{L(\lambda)}{\lambda - \lambda_\nu} \frac{1}{L'(\lambda_\nu)} \exp(-x\lambda_\nu) .$$

Of course, the intention to have the minimum number of terms in Eq. (2) dominates. As follows from the expression for a_ν the function $L(\lambda)$ should be among the polynomials orthogonal with the weight $f(s)$ in order to provide this. Then Eq. (9) reduces to a formula of the Gaussian type. But, from the other hand, the expansion of the exponent should exist and it belongs to those the description of which begins with the words "If there exists such $L(\lambda)$ that ... ." However, by no means these conditions should hold jointly.

Meanwhile, such properties of $s(g)$ as monotony, continuity and limitedness, which follow from Eq. (7), make it possible to use the Gaussian, Chebyshev and similar formulas ensuring the efficiency of Eq. (8).

The issue is continued by one consequence more,

$$a_\nu = \frac{1}{\Delta\omega} \int_{\omega \in \lambda_{\nu-1} \le \kappa(\omega) \le \lambda_{\nu+1}} d\omega,$$

of the theory of Dirichlet series. The structure of this expression is similar to that of Eq. (7). However, again the stumbling block appears, which is in the necessity to seek the function $L(\lambda)$. Transition to Eq. (8) is mathematically rigorous way to eliminate this trouble.

The properties of $s(g)$ already discussed allow one to treat Eq. (6) as a transition to an "effective" line, which replaces the "array" of spectral lines in $\kappa(\omega)$. In fact, there appears certain basis for arranging the attempts (see, for example, the analysis in Ref. 30) to solve similar problem using only purely physical arguments. The existence of an effective line seriously simplifies the calculation of some radiation quantities.

Series of exponents enable one to see sufficiently fine features of the line periphery from the experimental data pertaining, referring in fact only, to the central part of a spectral line (what looks rather unexpectedly). It is shown in Ref. 3 that at some frequency shift $\delta\omega$ the Lorentzian line shape changes for the exponential decay. As follows from Eq. (7) these regions are inessential for $g(s)$ and, consequently, for the coefficients of the series (8). The quantity $\delta\omega$ itself depends on temperature and this function can be easily retrieved by comparing the data calculated when varying $\delta\omega$ with the experimental data on Q. The latter quantity is undoubtedly determined by the intervals corresponding to the central part of the line.

Theory of the series (2) provides as well the mathematical grounds for calculating b_ν and $k_\nu \equiv s(g_\nu)$ directly in terms of $F(x)$. It can be shown that the function $K(\lambda) = \prod(1 - \lambda / k_\nu)$ well suits for the role of $L(\lambda)$ in the expansion of the exponent that leads to the system of equations

$$\frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} \frac{K(\kappa(\omega)) \, d\omega}{\kappa(\omega) - k_\nu} = b_\nu \, K'(k_\nu)$$

for k_ν. The left-hand side can easily be written in terms of the "moments" ($m = 1, 2 ...$)

$$w_m = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} \kappa^{(m)}(\omega) \, d\omega = (-1)^m \frac{\partial^m F(x)}{\partial x^m} ,$$

and the derivatives are calculated using the function $F(x)$ after its analytical continuation. Pragmatic usefulness of such a procedure is in the fact that the climatic and geophysical applications require only the absorption function in the majority of cases and therefore it is more reliable to use the experimental data on this function.

The basic relation (7) is useful when seeking coefficients of the $F(x)$ expansion over orthogonal exponential functions $D_m = \sum_{m'} C_{mm'} \exp(-x \, \zeta_{m'})$, which is an efficient calculational method. Then, ζ_m are considered as parameters minimizing the error of representation of F in the form a sum of small number of terms. The orthogonality $\int_0^\infty D_m(x) \, D_{m'}(x) \, dx = \delta_{mm'}$ is a means to write $C_{mm'}$ in terms of ζ_m.

3. GENERALIZATIONS OF THE METHOD

Applications of the above method of the representation of the absorption function as a series of exponents to solve the problems of the atmospheric spectroscopy already mentioned are quite obvious.

a) Inhomogeneous medium. In this case Eq. (1) is changed for the expression

$$H = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} d\omega \, \exp\left(- \int_{(l)} dl' \, \kappa(\omega, l')\right), \qquad (l)$$

where $\int_{(l)} dl'...$ is a curvilinear integral over the ray path of the length l; κ is the function of l' because of the dependence of the absorption coefficient on thermodynamic parameters of the spatially inhomogeneous atmosphere.

To reduce H to the form (2) it is sufficient to replace τ by $x\,\tau$, then use Eq. (7) and assume that $x = 1$. Then

$$H = \sum_{\nu} b_{\nu} \exp\left(- \tilde{s}(g_{\nu}, l)\right),$$

$$\tilde{g}(s, l) = \frac{1}{\Delta\omega} \int_{\tau(\omega,\, l) \leq s;\; \omega \in [\omega',\omega'']} d\omega, \qquad \tilde{s}(g, l) = \tilde{g}^{-1}(g, l)$$

with b_{ν} defined as earlier.

These rigorous expressions make the problem of calculational simplifications of H to be purely mathematical. The most natural simplification is

$$H = \sum_{\nu} b_{\nu} \exp\left(- \int_{(l)} dl' \, s(g, l')\right),$$

when $s(g, l')$ is defined according to the procedure (7) for each l' The latter relation was lively discussed, however, only on the heuristic level.

As it appears now the widely spread technique of reduction to (1) (see Sect. 3a) well combines with the series of exponents, when the ray path passes through the inhomogeneous over height Z atmosphere (between Z_1 and Z_2) with the zenith angle θ. $P(Z)$ and $\Theta(Z)$ are the pressure and temperature, respectively. This is achieved by introducing of approximation

$$\tilde{\kappa}(\omega, Z) = \tilde{\kappa}(\omega, Z_0) \frac{P(Z)}{P(Z_0)} \left(\frac{\Theta(Z_0)}{\Theta(Z)}\right)^{\alpha} \equiv \tilde{\kappa}(\omega, Z_0)\, \xi(Z)$$

and using a substitution of x in Eq.(1) by the value proportional to $\sec\theta \int_{z_1}^{z_2} \xi(Z)\, \beta(Z)\, dZ$, where $\beta(Z)$ is

the partial pressure of the absorbing gas; α and Z_0 play the role of parameters, and $\kappa = \tilde{\kappa}\beta$.

b) Overlapping of the absorption bands of different gases. Now the absorption coefficient is $\kappa(\omega) = \sum_{n} \kappa_n(\omega)$ where the sum is taken over the gas mixture constituents. There are no principle problems here, it is quite sufficient to replace by the sum that has just been written.

Obviously, the calculational inconveniences are quite clear, namely, κ_n depends on the partial pressure of the corresponding gas and for each set of gases the calculation according to Eq.(7) with the present sum should be done again. It would be desirable if we could deal with $s_n(g)$, i.e., with the values (7) for a separate κ_n. Then the approximation

$$F(x) = \sum_{\nu} b_{\nu} \exp\left(- x \sum_{n} s_n(g_{\nu})\right)$$

seems to be quite reasonable. By its mathematical content it is close to that considered in Sect. 3a and it is derived in a similar way. (It is true that its reliability is a little bit lower). Note in addition that in both cases the fact is essential that b_{ν} are simply the numbers. This circumstance underlines certain mathematical advantages of the variant (8).

A more sophisticated variant is associated with the fact that, as in the case with a mixture of two gases, we sacrifice the monotony of the function (7) for the component with lower absorption ($n = 2$, for the sake of certainty).

Let us introduce $z(g)$ instead of $s_2(g)$ into the relation similar to Eq. (6)

$$\tilde{F}(x_1, x_2) = \int_{0}^{1} dg \, \exp\left(-x_1\, s_1(g) - x_2\, z(g)\right).$$

Here $x_{1,2} = \beta_{1,2}\, x$, $\beta_{1,2}$ are partial pressures of gases in the mixture (of course the change for to $\tilde{\kappa}$ is assumed to be done). As to $z(g)$, the variation problem is formulated: the difference between $\tilde{F}$ and F is minimized in the sense of the least squares method under additional condition of transition to the rigorous variant at $x_1 = 0$. As it appears, the function $z(g)$ takes its maximum value, and its position is a good parameter for fitting.

c) Source function. The quantity called the source function is, by the definition,

$$S = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} d\omega \, B(\omega) \exp\left(x\, \kappa(\omega)\right)$$

with some quantity B. Most often the derivative of the Planck function with respect to the temperature is considered as a source function and is used in the

problem on fluxes of the infrared radiation in the atmosphere. (Usually $x\kappa \to \tau$, as in Sect. 3a, and then the corresponding corrections are needed). In other version, it could be the instrumental function as for example in spectroscopic measurements.

The exact expansion of S into a series over the exponents has the form (8) where $s(g_v)$ is replaced by

$$s_u(g_v), \quad s_u = g_u^{-1}(g),$$

$$g_u(s) = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''}$$

$$d\omega \, u(\omega) \, h(\omega) \,, \qquad h(\omega) = \begin{cases} l, & \kappa(\omega) \le s, \\ 0, & \kappa(\omega) > s \end{cases}$$

$$u(\omega) = B / \tilde{B} \,, \qquad \tilde{B} = (\Delta\omega)^{-1} \int_{\omega'}^{\omega''} B(\omega) \, d\omega \,, \text{ and in front}$$

of the sum (8) the quantity $\tilde{B}$ should be written.

The relation written for g_u can again be used when seeking purely calculational approximations. The variant $g_u \cong y(s)g(s)$ with the previous expression (7) and

$$y(s) = \frac{1}{s \, \Delta\omega} \int_{\omega_1(s)}^{\omega_2(s)} u(\omega) \, d\omega \,;$$

$$\omega_1(s) = \omega' + (1/2) \, (1 - s/s') \,,$$

$$\omega_2 = \omega'' - (1/2) \, (1 - s/s') \,.$$

seems to be a reliable one.

4. TRANSFER EQUATION FOR QUANTITIES INTEGRATED OVER FREQUENCY IN THE AEROSOL-MOLECULAR MEDIUM

Let $I(\mathbf{p}, \mathbf{r}, \omega)$ be the spectral intensity of a ray at the point $\mathbf{r}$ in the direction along the unit vector $\mathbf{p}$. The transfer equation has the form

$$\mathbf{p} \text{ grad } I = - (\sigma(\mathbf{r}) + \kappa(\mathbf{r}, \omega)) \, I(\mathbf{p}, \mathbf{r}, \omega) +$$

$$+ \int d\mathbf{p}'(\mathbf{r}, \mathbf{p}, \mathbf{p}') \, I(\mathbf{r}, \mathbf{p}', \omega) + \eta(\omega, \mathbf{r}) \,. \qquad (10)$$

In Eq.(10) φ is the scattering phase function, σ and η are the coefficients of the aerosol attenuation and total emission; $\eta = \eta^{(1)} + \eta^{(2)}$, where the components refer to the aerosol and to molecules, respectively.

The quantity

$$A(\mathbf{r}, \mathbf{p}) = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} I(\mathbf{r}, \mathbf{p}, \omega) \, d\omega \,, \qquad (11)$$

is necessary and the aerosol parameters φ, σ, and $\eta^{(1)}$ can be considered constant within the interval $\Delta\omega$.

An ingenious way of simplifying the problem (10) and (11) is suggested in Ref. 20. The series of exponents play there the role though not the primary but very essential. However, this solution is valid only for a homogeneous medium without the emission and necessary generalizations lean upon new elements discussed in this paper.

As it appears, one cannot do without small approximations. The first of them is the inequality

$$\frac{1}{\sigma^2} \text{ grad } \kappa(\mathbf{r}, \omega) \ll 1 \,,$$

which is almost unquestionable in many applications of the atmospheric optics. The second one is in practically inevitable use of approximations with $s(g, l)$ in the form of a series of exponents for an inhomogeneous molecular medium.

For Eq. (10) $I = I^{(0)} + I'$; $I^{(0)}$ is the solution of the homogeneous problem ($\eta = 0$ in Eq.(10)) with the boundary condition standard for the transfer problem and associated with the light coming from outside through the surface of a volume occupied by the medium; I' is a partial solution of the inhomogeneous equation with the "free" term η and with the zero boundary condition associated with the natural radiation of the medium. The quantity (11) finally takes the form $A = \sum_v b_v A_v$ with the ordinates of quadrature formulas b_v, the same as in all previous expressions. In accordance with the structure of the intensity $A_v = A_v^{(0)} + A_v'$. Let us write the results of calculations of terms in the last relations.

The quantity $A_v^{(0)}$ is the solution of equation (10) with the boundary condition $\eta = 0$, and, what is most important, with the molecular absorption coefficient κ selective over frequency replaced by the number $s(g_v, \mathbf{r})$ calculated following Sect. 3a, with $\mathbf{r}$ as a parameter.

Moreover, there appears a possibility of removing the second of the above-mentioned approximations (true, in a heuristic way) using the substitution of $s(g, \mathbf{r})$ for $\mathbf{p}$ grad $\tilde{s}(g, \mathbf{r})$, where $\tilde{s}$ is the exact variant from Sec. 3, (a) for $\tau = \int_0^\infty (\omega, \mathbf{r} - \mathbf{p} R) \, dR$. Similar action is also possible when constructing the solution of the inhomogeneous equation.

Then we have that, $A_v' = A_v^{(1)} + A_v^{(2)}$ in accordance with the earlier noted splitting of the radiation coefficient. The first term is the partial solution of Eq. (10), in which $\eta \to \Omega(\mathbf{r}) \, C$, $\kappa \to \gamma(g_v, \mathbf{r})$, $\Omega = (\Delta\omega)^{-1} \int_{\omega'}^{\omega''} B \, d\omega$ with the Planck function B, C is the aerosol absorption coefficient, γ denotes the function s_u from Sect. 3c at a certain $\mathbf{r}$. When calculating the

second term, the quantity $\Omega\gamma$ naturally appears instead of η (the other substitutions have already been described). However, the necessity is not excluded to replace B by $b\rho$, where the factor ρ describes the violation of the local thermodynamic equilibrium (for example, in the upper layers of the atmosphere or in the very far wings of the absorption bands[31]).

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