Construction of exponential series directly from information on the transmission function

S.D. Tvorogov

Institute of Atmospheric Optics,
Siberian Branch of the Russian Academy of Sciences, Tomsk

Received July 16, 2001

The possibility of expansion of the transmission function P into a series of exponents using directly the empirical (or some other) information on the spectrally integrated value of P is discussed. This approach does not require complicated calculation of the spectral molecular absorption coefficient connected with numerous approximations, empirical constants, and computational problems.

1. Formulation of the problem

Representing the transmission function

$$P(x) = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} e^{-x\kappa(\omega)}\, d\omega, \quad \Delta\omega = \omega'' - \omega' \qquad (1)$$

for the "dimensionless" thickness x of a layer of an absorbing gas with the molecular absorption coefficient $\kappa(\omega)$ for radiation at the frequency ω in the form of an exponential series

$$P(x) = \int_0^1 e^{-xs(g)}\, dg = \sum_\nu b_\nu\, e^{-xs(g_\nu)} \qquad (2)$$

(where b_ν and g_ν are ordinates and abscissas of the corresponding quadrature formula) has, for a long time, been a popular trick in solving problems of atmospheric spectroscopy.[1–3] The function $s(g)$ in Eq. (2) inverse to

$$g(s) = \frac{1}{\Delta\omega} \int d\omega, \quad \kappa(\omega) \le s; \omega \in [\omega', \omega''] \qquad (3)$$

and exact in Eq. (3) follows from

$$g(s) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{dx}{x} P(x)\, e^{sx} = \int_0^s f(s)\, ds;$$
$$f(s) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dx\, e^{sx} P(x); \quad c > 0. \qquad (4)$$

Equations (4) are obvious corollaries of the initial definitions of f and g:

$$P(x) = \int_0^\infty f(s)\, e^{-sx} ds, \quad \frac{P(x)}{x} = \int_0^\infty g(s)\, e^{-sx} ds. \qquad (5)$$

In principle, Eq. (3) solves the problem on constructing the series (2), but calculation of $\kappa(\omega)$ invokes numerous approximations including great number of empiric parameters. In essence, for the transmission function (1) as a spectrally integrated parameter, many spectral features of $\kappa(\omega)$ are insignificant. Therefore, it is desirable to construct $g(s)$ directly from the information on $P(x)$. The initial information may be empirical data or their approximations either direct or relying on the models of absorption bands.

However, one cannot make use of Eq. (4) in computations, because numerical construction of an analytical extrapolation of an empiric function seems to be unrealistic. Approximations, in their turn, usually include $\sqrt{x}$ (there are some physical reasons for this[4]). At a similar extrapolation, this will lead to bifurcation of solutions with unclear mathematical corollaries.

Certainly, Eqs. (5) can be treated as integral equations for f and g, but solution of the ill-posed inverse problem is difficult because of the empirical origin of Eq. (1). Further, $P(x)$ depends on thermodynamic characteristics of the medium, and every time at their variations, one has to solve Eq. (5) anew. In addition, significant difficulties arise at generalization of Eq. (2) to the case of an inhomogeneous medium, beam overlapping, calculation of the source function.[3]

Therefore, it is desirable to find such a version that

$$g(s) = \int_0^\infty P(x)\, \Phi(x; s)\, dx \qquad (6)$$

with Φ obeying some, independent of P, equation. The proof of the existence of Eq. (6) is considered in this paper.

2. Analytical properties of $P(z)$ with complex $z = x + iy$

From the definition (1) it follows that $P(z)$ is an integer function with the properties

$$\lim_{|z|\to\infty} |P(z)| = 0; \; x \ge 0; \quad \lim_{|z|\to\infty} |P(z)| = \infty, \; x < 0\,.$$

At the imaginary axis

$$P(iy) = U(y) + iV(y);$$

$$\begin{Bmatrix} U \\ V \end{Bmatrix} = \frac{1}{\Delta\omega} \int_{\omega'}^{\omega''} d\omega \begin{Bmatrix} \cos[y\kappa(\omega)] \\ \sin[y\kappa(\omega)] \end{Bmatrix} \quad (7)$$

with even $U(y)$ and odd $V(y)$.

These properties of $P(z)$ allow us to shift integration in Eq. (4) to the imaginary axis ($c \to 0$). Using a standard approach, we derive the dispersion equations

$$U(y) = \frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{V(y')\,dy'}{y - y'},\; V(y) = -\frac{1}{\pi} P \int_{-\infty}^{+\infty} \frac{U(y')\,dy'}{y - y'}. \quad (8)$$

3. Transition to Eq. (6)

Substituting Eq. (7) into Eq. (4), where $c = 0$, and then excluding V by Eq. (8) and using the symmetry properties of U and V, we obtain

$$g(s) = \frac{2}{\pi} \int_0^\infty dy\, U(y) \frac{\sin sy}{y}. \quad (9)$$

Naturally, after substitution of Eq. (7) into Eq. (9), turn back to Eq. (3).

Consider the integral

$$I = \frac{1}{2\pi i} \int_C \frac{P(z)\,dz}{z - x} = P(x)$$

over the contour C shown in Fig. 1. The properties of $P(z)$ from Section 2 lead to the following equation:

$$P(x) = \frac{2x}{\pi} \int_0^\infty \frac{U(y)\,dy}{y^2 + x^2}. \quad (10)$$

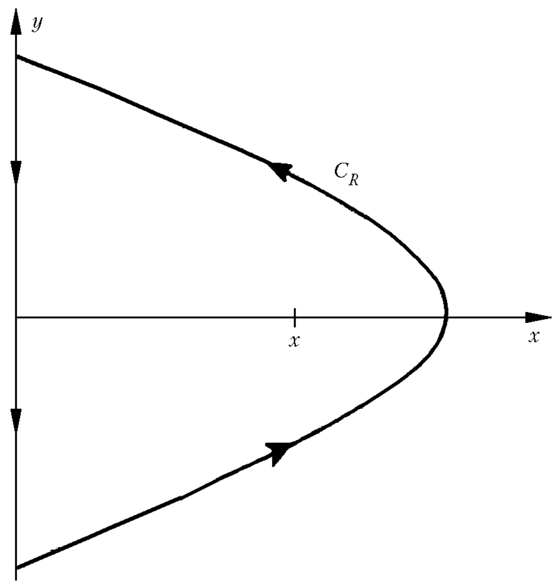

Fig. 1. The integration contour used in deriving Eq. (10); C_R is a crescent of radius $R \to \infty$.

Certainly, Eq. (10) can be treated as an equation for $U(y)$ and then $g(s)$ can be calculated by Eq. (9). However, we can see that, mathematically, this version reduces to the already discussed equation (5).

Then, seemingly, it is worth trying to express $P(iy)$ through $P(x)$ using the idea of the Schwartz integral for a half-plane.[5] Here we have to consider the integral (with the complex variable $\xi = t + i\tau$)

$$I_1 = \frac{1}{\pi} \int_C \frac{P(\xi)\,d\xi}{(x - \xi)^2 + y^2} = P(z)$$

over the contour C (Fig. 2). Simply writing the integrals over the axes t and τ, we obtain the equation

$$P(x + iy) = \frac{1}{\pi} \int_0^\infty \frac{y\,P(t)\,dt}{(x - t)^2 + y^2} - \frac{1}{\pi} \int_0^\infty \frac{iyP(i\tau)\,d\tau}{(x - i\tau)^2 + y^2}. \quad (11)$$

The first term is a harmonic function taking the value $P(x)$ at the real axis ($y \to 0$). Another integral is the difference from the desirable function. (Although it is zero at $y \to 0$.)

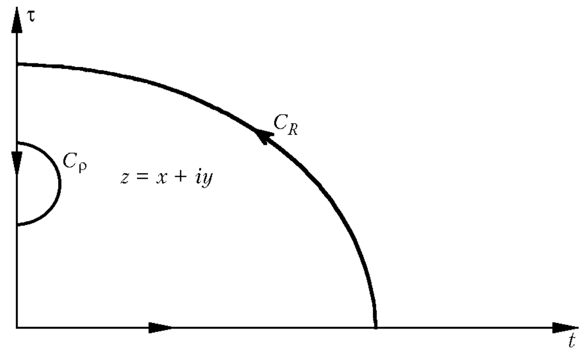

Fig. 2. Integration contour used in deriving Eq. (11): C_ρ is a crescent of radius $\rho \to 0$.

In the considered version, at $x \to 0$ the contour in Fig. 2 is to be deformed by passing around the point $\tau = y$ by the crescent of radius $\rho \to 0$. Then, we have the integral equation (Fredholm integral equation of the first kind)

$$P(iy) = \frac{2}{\pi} \int_0^\infty \frac{P(t)\,y\,dt}{t^2 + y^2} - \frac{2i}{\pi} \int_0^\infty P \frac{y\,P(i\tau)\,d\tau}{y^2 - \tau^2}$$

for $P(iy)$ with a “free” term expressed through Eq. (1). Again the direct check shows that solution of the latter equation is Eq. (7), that is, we again come back to the problems already discussed in Section 1.

The version (6) excluding the above computational difficulties results from a simple formal transformation. Assume that $\Phi(x; s)$ exists as a solution of the integral equation (Fredholm integral equation of the first kind)

$$\int_0^\infty \frac{x\,\Phi(x; s)\,dx}{y^2 + x^2} = \frac{\sin sy}{y}. \quad (12)$$

Then, multiplying Eq. (10) by Φ, integrating over x, and applying Eq. (9), we immediately come to Eq. (6).

Note here that the transition from Eqs. (9), (10), and (12) to Eq. (6) naturally assumes the permutability of the integrals in the relation

$$\int_0^\infty \mathrm{d}x\, x\, \Phi(x;s) \int_0^\infty \frac{U(y)\,\mathrm{d}y}{y^2+x^2}.$$

This problem (as in all other cases) is solved by the standard methods.[6]

It is clear that Eq. (12) is independent of thermodynamic parameters and possible variations of the function (1) – all the corresponding characteristics of g(s) arise already after substitution of the "proper" P quantity into Eq. (6). (Inhomogeneous medium, band overlapping, source function.[3])

After multiplication of Eq. (12) by cos ξy and the operation $\int_0^\infty \mathrm{d}y(\ldots)$, we see that

$$\int_0^\infty \Phi(x;\xi)\, \mathrm{e}^{-\xi x}\, \mathrm{d}x = \begin{cases} 1 & \xi < s \\ \frac{1}{2} & \xi = s \\ 0 & \xi > 0 \end{cases} = \tag{13}$$

$$= \frac{1}{2\pi} \int_{c-i\infty}^{c+i\infty} \frac{\mathrm{d}\rho}{\rho}\, \mathrm{e}^{\xi\rho}\left(1 - \mathrm{e}^{-s\rho}\right).$$

Then, if we assume that Φ is a solution to Eq. (13), then Eqs. (6) and (1) lead to the exact Eq. (3).

4. Mathematical aspects concerning the Eqs. (6), (12), and (13)

The Fredholm integral equations of the first kind have some fine mathematical aspects (see, for example, Ref. 7). The central problem is uniqueness of the solution of Eqs. (12) or (13). However the benchmark is Eq. (10), and its unique solution is Eq. (7) what can be directly checked. Other transformations accompanied by clarification of the possibility to permute integrations are identical. Certainly, here we need an additional phrase that P has a mathematical structure (1).

The following solution of Eq. (12) or (13) should likely be only numerical, and this assumes invoking of the corresponding and non-trivial[8] tricks (by the way, if we aim at V instead of U, then in Eq. (6) $\Phi \to \psi$, and the latter satisfies the equation

$$\int_0^\infty \frac{\psi(x;s)\,\mathrm{d}x}{y^2+x^2} = \frac{1}{y^2}(1-\cos sy)$$

with the always positive right-hand side. In this case $\partial\psi/\partial s = x\Phi$).

It may appear possible to write an analytical equation for Eq. (12). Actually, assume that Φ is regular in the right half-plane z. Then, transforming Eq. (6) by contour integration as shown in Fig. 2, express g(s) through the integral over the imaginary axis. Then, writing Eq. (9) in the equivalent form

$$g(s) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}y\, \frac{\sin sy}{y}\, U(y) - \frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}y\, \frac{1-\cos sy}{y}\, V(y),$$

we find an explicit form of Φ at the imaginary axis, and it only remains for us to extrapolate it to the positive real axis. However, this scenario is impossible, what became clear, in fact, when discussing Eq. (11), because it is formally equivalent to transformation of the upper half-plane into the right-hand side one, but in this case there is no any harmonic function corresponding to the Schwartz integral for a half-plane. In other words, the initial assumption about Φ is not true.

Then, solving Eq. (13), we, seemingly, should use the inverse Laplace transformation, but it is possible only if the right-hand side of the equation is a function regular in the right half-plane[9]; however, it is not the case with Eq. (13) because of discontinuity of the derivative. Certainly, this does not mean that Eq. (13) has no solution; this only means that the solution cannot be found through the inverse Laplace transformation.

Further simplification of Eqs. (6) and (13) is possible. Assume that in Eq. (12) we have $\Phi(x;\, s) = s\varphi(x;\, s)$, $x = y\eta$, $sy = a$, then

$$\int_0^\infty \frac{\eta\varphi(y\eta;\, s)\,\mathrm{d}\eta}{1+\eta^2} = \frac{\sin a}{a}.$$

Now the statement that φ depends on the product $y\eta s = a\eta$ looks rather reliable. If we also take that $a\eta = q$, then we derive the equation

$$\int_0^\infty \frac{q\,\varphi(q)\,\mathrm{d}q}{a^2+q^2} = \frac{\sin a}{a}.$$

The following transformations are the same as at transition from Eqs. (12) and (13), and the result is the equation

$$\int_0^\infty \varphi(x)\, \mathrm{e}^{-\xi x}\mathrm{d}x = \begin{cases} 1 & \xi < 1, \\ \frac{1}{2} & \xi = 1, \\ 0 & \xi > 1. \end{cases} \tag{14}$$

Equation (6) after the above transformations acquires the form

$$g(s) = \int_0^\infty P\left(\frac{x}{s}\right)\varphi(x)\,\mathrm{d}x \tag{15}$$

with the solution in the form of Eq. (14).

From Eq. (15), the correct statement $\lim_{s\to\infty} g(s) = 1$ corresponding to Eq. (3) follows. Actually, $\lim_{s\to\infty} P(x/s) = P(0) = 1$ in view of Eq. (1), and $\int_0^\infty \varphi(x)\,\mathrm{d}x = 1$. Then, $\lim_{s\to 0} P(x/s) = P(\infty) = 0$, and, according to Eq. (15), $\lim_{s\to 0} g(s) = 0$, as is needed for Eq. (3). Correspondingly, equation (3) itself is the corollary of Eqs. (15), (1), and (14).

Acknowledgments

The work was partially supported by Russian Foundation for Basic Research Grant No. 00–05–65209.

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