REPRESENTATION OF THE TRANSMISSION FUNCTION BY THE SERIES OF EXPONENTS

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The representation of the transmission function by the series of exponents is discussed based on the idea of replacing the absorption coefficient very changeable with frequency by a smooth function of frequency. Making use of this representation, simple approximations of the transmission function are derived for inhomogeneous media and overlapping spectra. The adequacy of these relations is illustrated by calculations of the transmission function in the spectral ranges $6600-7700$ cm^{-1} and $2200-2400$ cm^{-1} and by their comparison with experimental data.

The method referred to as the k-distribution or the series of exponents is such a trick by which the absorption coefficient $\varkappa(\omega)$, entering into the expression for the transmission function $F(z)$ (in the frequency range $\Delta\omega = \omega'' - \omega'$ for an equivalent absorber amount z) and grossly changing with frequency ω, is replaced by a monotonic function with $s(g)$ (an example of $\varkappa(\omega)$ juxtaposed $s(g)$ is shown in Fig. 1). Replacement is performed in such a manner that the equality

$$F(z) \equiv \frac{1}{\Delta\omega} \int e^{-z\,\varkappa(\omega)}\, d\omega = \int_0^1 e^{-z\,s(g)}\, dg \qquad (1)$$

is perfectly exact. Furthermore, in the second equality of Eq. (1) the quadrature formula (with abscissas g_n and ordinates a_n) is applied, which in essence marks the appearance of the series of exponents

$$F(z) = \sum_n a_n\, e^{-z\,s(g_n)} \qquad (2)$$

with, naturally, small number of terms.

The utility of this trick with series (2) in calculating the characteristics of an aerosol−molecular medium integrated over the frequency spectrum is well known.[1] At present, this idea is widely applied[2−16] for solving conventional problems of atmospheric spectroscopy (calculation of F for an inhomogeneous medium, overlapping spectra, and the source function). However, it is only one of the procedures used for this purpose, and by no means most efficient. The potentialities and advantages of the method discussed are most likely not exhausted but they need to be proved and argued. Some mathematical and methodical foundation is necessary for this purpose. In what follows some considerations related to this sufficiently general problem and their concrete illustrations are presented.
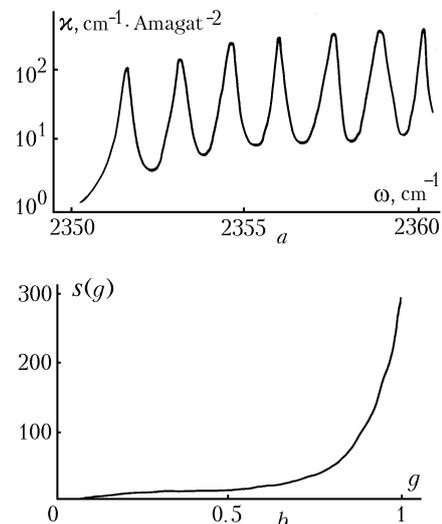

FIG. 1. *Absorption coefficient of* CO_2−N_2 *in the spectral range* $2350-2360$ cm^{-1} *at* $T = 300$ K *(a) and function* $s(g)$ *inverse to* $g(s)$ *in the same spectral range (b).*

Let us first note that the way of realization of Eq. (1) is the Laplace transform and the list of usually applied starting relations is well known

$$F(z) = \int_0^\infty f(s)\, e^{-sz}\, ds \, ,$$

$$f(s) = \frac{1}{2\pi i} \int_{h-i\infty}^{h+i\infty} dz\, e^{sz}\, F(z) \, , \quad h > 0, \qquad (3)$$

$$g(s) = \int_0^s f(s)\, ds \, , \quad g(s) = \frac{1}{2\pi i} \int_{h-i\infty}^{h+i\infty} dz\, \frac{F(z)}{z}\, e^{sz} \, , \qquad (4)$$

where $s(g)$ is the function reverse to $g(s)$ from Eq. (4).

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The first methodical point is initiated by Refs. 17–19, where the series in the form of Eq. (2), being the Dirichlet series according to the terminology presently accepted in mathematics, are investigated at the mathematical level of rigor. This creates that "mathematical climate" which enables one to circumvent the prevailing reasoning at the "physical level of rigor" in Refs. 2–16 accompanied with phrases rather verbose and sometimes appealing to pure intuitive considerations.

A detailed example can be found in Ref. 20. It is related to calculating $s(g)$ and $g(s)$ immediately from $\varkappa(\omega)$, in actuality, from the spectroscopic databases. It is apparent that the answer should be obtained by substituting the first equality of Eq. (1) in Eq. (3) or (4) with subsequent change of the order of integration over ω and z. However, as it appears, this operation is mathematically possible only for Eq. (4) and results in a rather simple calculating procedure

$$g(s) = \frac{1}{\Delta\omega} \int\limits_{\varkappa(\omega)\le s,\ \omega\in[\omega',\omega'']} d\omega .$$ (5)

The consequence of this fact is very remarkable. The first expression in Eq. (3) can be surely written as a quadrature formula

$$F(z) = \sum_n b_n\, e^{-s_n z}$$ (6)

with abscissas s_n and ordinates b_n. However, in spite of the formal equivalence of Eqs. (2) and (6), the first formula should be preferred for the reason already given in the previous paragraph. This situation can be well classified as mathematical self-consistency because, on the other hand, a_n and g_n in Eq. (2) are "simply the numbers," whereas in Eq. (6) the ordinates b_n depend, of course, on the characteristics of the medium in view of their explicit relation to f.

The last circumstance is of primary importance when substantiating the approximate expedients of solving the problems of atmospheric spectroscopy. We bear in mind the fact that in Eq. (2) the parameters of the medium enter only into $g(s)$ by Eq. (5).

An analysis shows that for the inhomogeneous medium

$$F \equiv \frac{1}{\Delta\omega} \int\limits_{\omega'}^{\omega''} \exp\left[-\int\limits_{(l)} \varkappa(\omega, l)\, dl\right] d\omega =$$

$$= \sum_n a_n \exp\left[-\int\limits_{(l)} s(g_n, l)\, dl\right] d\omega \cong$$

$$\cong \sum_n a_n \exp\left[-\sum_j s(g_n, l_j)\Delta l_j\right] .$$ (7)

In Eq. (7), the curvilinear integral $\int dl(...)$ along the ray path appears, and $\varkappa$ is a function of the medium l in addition to ω. In the last equality in Eq. (7) $\int dl(...)$ is represented as an integral sum. An example illustrating the accuracy of Eq. (7) is given in Table I.

Similar estimates (and with obligatory appeal to Eq. (2)) assert a reasonable possibility of the approximation

$$F \equiv \frac{1}{\Delta\omega} \int\limits_{\omega'}^{\omega''} e^{-\varkappa_1 z_1 - \varkappa_2 z_2}\, d\omega = \sum_n a_n\, e^{-s_1(g_n)z_1 - s_2(g_n)z_2}$$ (8)

for the transmission function in the case of overlapping spectra. The symbols $\varkappa_1$ and $\varkappa_2$ are used for the absorption coefficients of gases in the mixture, z_1 and z_2 are the equivalent absorber amounts, and s_1 and s_2 are constructed with the use of Eq. (5) for each gas separately. The efficiency of Eq. (8) can be seen from Table II.

TABLE I. *Calculation of transmission by* H_2O *for inhomogeneous media*, 6622–7092 cm^{-1}, F_{lbl} = 0.262 *and* F_{expon} = 0.260.

Serial number of layer	F, K	P, atm	ρ_{H_2O}, g/m^3	$s_n(l)$	n				
					1	2	3	4	5
					a_n				
					0.118	0.239	0.284	0.239	0.118
1	291	0.962	9.33	$s_n(l_1)$	0.028	0.214	0.770	3.184	23.83
2	289	0.913	7.95	$s_n(l_2)$	0.022	0.175	0.631	2.611	20.14
3	287	0.863	6.77	$s_n(l_3)$	0.017	0.141	0.514	2.140	17.04
4	281	0.768	4.96	$s_n(l_4)$	0.011	0.092	0.339	1.435	12.15
5	269	0.592	2.09	$s_n(l_5)$	0.009	0.031	0.114	0.503	4.76
$a_n \exp\left(-\sum_i s_n(l_i)\right)$					0.108	0.124	0.0264	10^{-5}	–

TABLE II.   Calculation of transmission by H_2O+CO_2 for overlapping spectra, 6622–7092 cm^{-1}, T = 296 K, P = 1 atm, P_{CO_2} = 3·10^{-4} atm and ρ_{H_2O} = 10^{-2} g/m^3.

k	1	2	3	4	5	l, km	F_{expon}	F_{lbl}	$\dfrac{F_{expon}}{F_{lbl}}$
a_n	0.118	0.239	0.284	0.239	0.118	1	0.995	0.993	1.002
$s_n^{(1)}$	3.24·10^{-5}	2.39·10^{-4}	8.55·10^{-4}	3.54·10^{-3}	2.60·10^{-2}	10	0.952	0.938	1.014
$s_n^{(2)}$	–	0	1.05·10^{-5}	3.17·10^{-4}	1.07·10^{-2}	100	0.779	0.773	1.06
						1000	0.428	0.371	1.15

Table III allows one to estimate the number of terms in Eq. (2) if the Gauss or Chebyshev quadrature formulas are used. In addition we note that in the direct line-by-line calculation of F by Eq. (1), ~60 thousands of points should be used.

TABLE III.   Calculation accuracy of transmission by CO_2+H_2O using   the   series   of   exponents, 7092–7634 cm^{-1}, T = 296 K, P = 1 atm, ρ_{H_2O} = 10 g/m^3, and P_{CO_2} = 3·10^{-4} atm.

l, km	0.004	0.05	0.5	1	5
F_{lbl}	0.918	0.680	0.370	0.298	0.167
F_{Gauss5}	0.921	0.682	0.373	0.309	0.171
F_{Gauss6}	0.917	0.680	0.364	0.289	0.170
F_{Gauss7}	0.916	0.678	0.373	0.302	0.160
F_{Ch6}	0.926	0.682	0.374	0.296	0.147
F_{Ch7}	0.924	0.683	0.372	0.300	0.159
F_{Ch9}	0.920	0.682	0.370	0.303	0.172
F_{Gauss5}/F_{lbl}	1.003	1.004	1.009	1.037	1.026
F_{Gauss6}/F_{lbl}	0.9987	0.9999	0.985	0.970	1.020
F_{Gauss7}/F_{lbl}	0.9975	0.9981	1.008	1.013	0.961
F_{Ch6}/F_{lbl}	1.009	1.003	1.012	0.994	0.882
F_{Ch7}/F_{lbl}	1.007	1.004	1.007	1.005	0.950
F_{Ch9}/F_{lbl}	1.002	1.003	1.002	1.017	1.031

Another methodical point consists in our conviction that when constructing radiation blocks for climate models and algorithms for geophysical applications, the reliability of suggested approaches should be checked by comparison of the appropriate estimates with experimental data. Figures 2 and 3 show examples of our calculations.
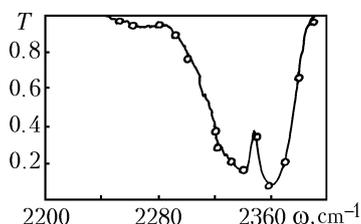

FIG. 2.   Transmission function in the spectral range 2200 − 2400 cm^{-1}. Curve shows experimental data of Ref. 22 and dots are for the results of our calculation using the series of exponents that coincide with the line−by−line calculation at the scale of the figure. Here T = 291 K, P = 6.21·10^4 Pa, and P_{CO_2} = 0.0230.
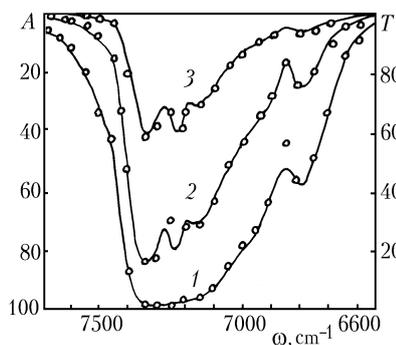

FIG. 3.   Transmission spectrum of H_2O within the 1.4 μm band.   Curves show the experimental data,[23] dots are for the results of calculation using the series of exponents, u is the equivalent amount of the water vapor,   u = 0.845 (1), 0.135 (2), and 0.018 g/cm^2 (3), and P = 1 atm.

The position described above pays some unexpected dividends, namely, the possibility to judge on the line shape periphery from its resonance part. The matter is that when using Eq. (5) for calculations, the function $g(s)$ is surely determined by the regions corresponding to the line centers, and the line wings with their exponential decrease[21] can be ignored. Therefore, the calculation is performed using the Lorentzian line shape truncated at that displacement from the line center at which the periphery begins. This boundary, as it appears from comparison between experimental and calculated data, varies with the temperature.

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