SOME APPLICATIONS OF THE EXPONENTIAL SERIES FOR CALCULATING THE ABSORPTION FUNCTION

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The possibilities of quickly calculating the transmission function using the Dirichlet series are discussed. Such a technique should provide an insight into the solution of pragmatic problem on reducing the volume of radiation codes in climatic models and geophysical applications of the atmospheric spectroscopy.

The expression for the transmission function

$$P(x) = \frac{1}{\Delta\omega} \int\limits_{\omega'}^{\omega''} \mathrm{d}\omega \exp(-\varkappa(\omega)x) \qquad (1)$$

with the spectral (for frequency ω and $\Delta\omega = \omega''-\omega'$) coefficient of molecular absorption $\varkappa(\omega)$ and the argument x (for example, by the precipitated layer of absorbing gas), with the use of exponential series, can be rearranged to the form

$$P(x) = \int\limits_0^\infty f(s)\mathrm{d}s = \int\limits_0^1 \mathrm{d}g \exp(-s(g)x) \qquad (2)$$

with a subsequent application, to Eq. (2), of the suitable formula of integration. In Eq. (2) $f(s)=g'(s)$; $s(g)$ is the function inverse to $g(s)$; and, as was shown in Ref. 1,

$$g(s) = \frac{1}{\Delta\omega} \int\limits_{\varkappa(\omega)\le s,\ \omega\in[\omega'',\omega']} \mathrm{d}\omega. \qquad (3)$$

The formulation of the problem considered below is rather natural. Let us assume that the function (3) is constructed for the "base" (say, 10 cm^{-1} wide) intervals $\delta\omega$, and it is necessary to calculate, from these data, Eq. (1) for random $\Delta\omega > \delta\omega$. The principal answer is obvious: because of Eq. (3) we have

$$g(s) = \sum_{\alpha=1}^{\beta} g^{(\alpha)}(s) \frac{\delta\omega_\alpha}{\Delta\omega}, \qquad (4)$$

where α is the number of an interval in $\Delta\omega$ division into β portions (and for some reasons $\delta\omega$ can be different), and $g^{(\alpha)}(s)$ is the function (3) for the corresponding "elemental" spectral range.

The following refinement of the problem is connected with the purely pragmatic reasons – the need to have, in the radiation codes, the least time- and space-expensive version, providing however suitable accuracy. Therefore it is desirable to refer to the function (3) directly related to $\varkappa(\omega)$ in order to exclude the recalculation of $s(g)$ after application of Eq. (4). For purely mathematical reasons (see Ref. 1), differentiation of $g(s)$ is only possible by numerical methods. Integration by part in the first expression (2) reduces $P(x)$ to the form

$$P(x) = \exp(-xs_{\max}) + x \int\limits_{s_{\min}}^{s_{\max}} \mathrm{d}s\, g(s)\exp(-sx), \qquad (5)$$

and the existence of the portion $s_{\min} \le s \le s_{\max}$, where $s_{\max}$ and $s_{\min}$ are the maximum and minimum values of $\varkappa$ at the interval considered, is the direct consequence of Eq. (3).

If one uses most rational formulas of integration, the integration over a fixed interval (usually, [0, 1]) of a dimensionless variable should be used. Certainly, there is no such integration in the combination of equations (5) and (6). The method to be used is rather simple – the change of variable

$$s = \lambda(s_{\max} - s_{\min}) + s_{\min},\quad 0 \le \lambda \le 1, \qquad (6)$$

reduces the integral from Eq. (5), at any spectral interval, to

$$\sum_{j=1}^{n} g\Big(\tilde{s}(\lambda_j)\exp[-\tilde{s}(\lambda_j)]\Big) a_j \qquad (7)$$

with simple numbers λ_j and a_j, determined by the chosen formula of integration, where some nth degree polynomial takes part.

However, there is one fine detail while very important. The point is that within practically any spectral range intensities of spectral lines vary by several orders of magnitude and similar great difference will take place between $s_{\min}$ and $s_{\max}$. This, in turn, results in the fact that after the variable substitution (6) a marked portion of the curve $g(s)$ simply drops out from consideration that is the cause of a great error in calculations.

TABLE Ix

j	0λ	s	g
1	0.058069	23.576	0.78
2	0.23517	95.479	0.92
3	0.33804	134.16	0.95
4	0.5	203	0.97
5	0.66195	268.75	0.98
6	0.76483	310.5	0.99
7	0.94193	382.42	0.994

TABLE IIx

x	P	
	Calc. by Eqs. (4) and (5)	Exact calculation
0.001	0.865	0.863
0.1	0.428	0.564
1	0	0.325

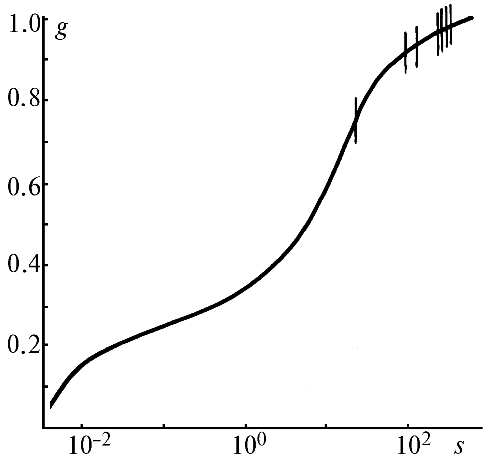

FIG. 1. Bars on the curve $g(s)$ denote s values corresponding to Eq. (7).

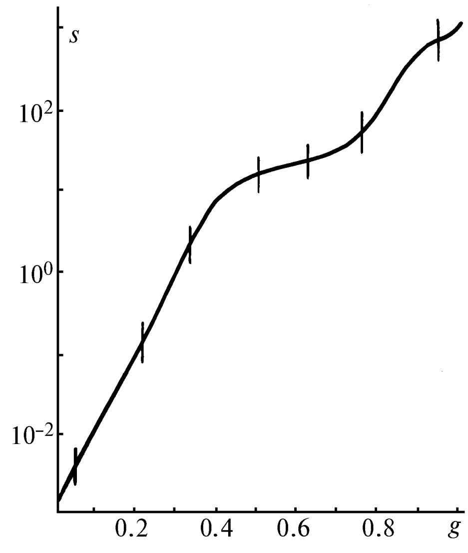

FIG. 2. Uniform distribution of abscissas in Eq. (2).

The situation for the 2350–2400 cm^{-1} range of the CO_2 spectrum is illustrated by Tables I and II and Fig. 1 for the case when Eq. (5) corresponds to the Chebyshev formula of integration (ordinates $a_j = 1/n$ and below $n = 7$). In the case under consideration $s_{\min} = 1.25\cdot 10^{-3}$ and $s_{\max} = 407$. For a comparison, Fig. 2 shows how all information on Eq. (3) is used when applying the second expression (2).

As we have found out, the technical difficulty we faced can be removed rather simply and efficiently. It turns out to be possible to calculate the integral from Eq. (5) (accurate to no less that 2–3%) following the scheme

$$\int\limits_{s_{\min}}^{s_{\max}} \mathrm{d}s \to \int\limits_{s_1}^{s_2} \mathrm{d}s + \int\limits_{s_2}^{s_3} \mathrm{d}s + \ldots \int\limits_{s_{m-1}}^{s_m} \mathrm{d}s. \tag{8}$$

In Eq. (8) $s_1 = 10^{l_1}$ is the number closest to $s_{\min}$ under the condition $10^{l_1} < s_{\min}$, $s_2 = 10^{l_1+1}$, $s_3 = 10^{l_1+2}$ and so on up to $s_m = 10^{l_2}$ – the number closest to $s_{\max}$, and $s_m > s_{\max}$. The variable in Eq. (6) is now $s'_{\max}(0.9\lambda + 0.1)$ and the upper limit plays the role of $s'_{\max}$. The formulas (6) and (7) are then applied to each integral from Eq. (8), what involves all the information about $g(s)$ into the calculation of P.

The final expression

$$P = \sum_{j=1}^{n} \sum_{\alpha=1}^{\beta} \sum_{l=l_1}^{l_2} \frac{\delta\omega}{\Delta\omega} g^{(\alpha)}\big(10^l(0.9\lambda_j + 0.1)\big) \times$$
$$\times \exp\big[-x\big(10^l(0.9\lambda_j + 0.1)\big)\big] \tag{9}$$

will be the consequence of Eqs. (8), (4), and (7). It is just this expression that gives a solution to the above-formulated calculational problem.

Before discussing one more aspect of the exponential series, we would like to remind some points of the theory of Dirichlet series.[2–4] If s_j are zeros of the properly selected integral function $L(s)$, then

$$P(x) = \sum_j b_j \exp(-xs_j); \tag{10}$$

$$\sum_{j'}^{1} b_{j'} = \frac{1}{2\pi i} \sum_{c-i\infty}^{c+i\infty} \frac{\mathrm{d}z}{z} \mathrm{e}^{\eta z} P(z),\ c > 0,\ s_j < \eta < s_{j+1} x \tag{11}$$

If follows from Eqs. (11), (3), and (1) that in Eq. (10)

$$b_j = g(\eta) - g(\eta'),\ s_{j-1} < \eta < s_j , \tag{12}$$

where η has the same meaning as in Eq. (11).

Theoretically, η and η' can be selected in any way from the indicated intervals. But it will be so if the problem of $L(s)$ is exactly solved – for it the exponent expansion exists, the Dirichlet series converges, and just to its proper function.

However, in practice in Eq. (10), as well as in Eq. (7), the finite-degree polynomial will take place in spite of L. And, as follows from Eq. (12), it should enter into the set of polynomials orthogonal with the weight $f(s)$ at the interval $[s_{\min}, s_{\max}]$. The construction of such a function is a rather cumbersome process and certainly we have to restrict our consideration to standard formulas of integration, when the role of s_j is played by their abscissas. Therefore the choice of η and η′ should be considered as an approximation procedure.

Figure 3 illustrates schematically the problem arose. We should express $g(\eta)$ in terms of $g(s_j)$ in a reasonable way. The arithmetical averages of ordinates

$$b_1 = \frac{1}{2}(g_1 + g_2),\ b_2 = \frac{1}{2}(g_3 - g_1),\ b_3 = (g_4 - g_2)\ \ldots$$

$$b_j = 1 - \frac{1}{2}(g_{j-1} + g_j),$$

where $g_j = g(s_j)$, can be considered as a result. In other version, the result is the arithmetical averages of abscissas

$$b_1 = g\left(\frac{s_1 + s_2}{2}\right),\ \ b_2 = g\left(\frac{s_2 + s_3}{2}\right) - g\left(\frac{s_2 + s_1}{2}\right),$$

$$b_3 = g\left(\frac{s_3 + s_4}{2}\right) - g\left(\frac{s_3 + s_2}{2}\right),$$

$$b_{j-1} = g\left(\frac{s_{j-1} + s_j}{2}\right) - g\left(\frac{s_{j-1} + s_{j-2}}{2}\right),$$

$$b_j = 1 - g\left(\frac{s_j + s_{j-1}}{2}\right).$$

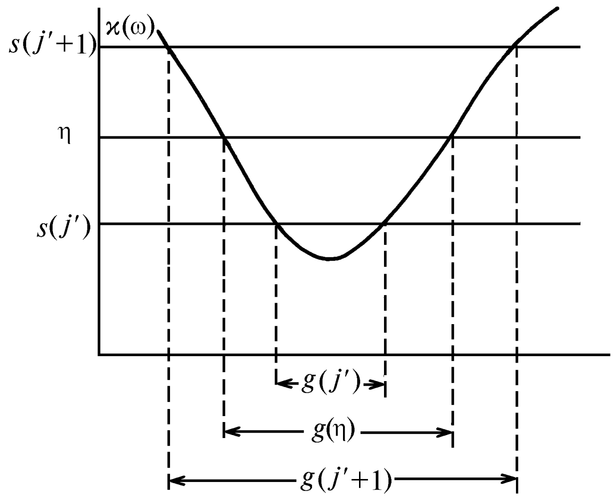

FIG. 3. Set out as an ordinate is $g(s)$ multiplied by $\Delta\omega$.

In any case, to apply Eq. (4), one should use the procedure like in formulas (5)–(9).

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