SOME ASPECTS OF THE PROBLEM OF REPRESENTATION OF THE ABSORPTION FUNCTION BY A SERIES OF EXPONENTS

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The problem of representation of absorption function by a series of exponents with the coefficients expressed directly in terms of characteristics of spectral lines is discussed.

1. ON CALCULATION OF SPECTRALLY INTEGRATED QUANTITIES

In discussion of a number of radiative problems the necessity arises to find a quantity $\tilde{G} = (1/\Delta\omega)\int\limits_{\omega'}^{\omega''} d\omega\, G(k(\omega))$ (ω is the frequency and $\Delta\omega = \omega'' - \omega'$ is the spectral interval), when the spectral optical density of a gas $\tau = \kappa\, l = k\, z$. Here $\kappa(\omega)$ is the molecular absorption coefficient (cm^{-1}), l is the distance travelled by a beam, z is the properly introduced dimensionless "length". The special, but important, example of the function $\tilde{G}$ is the transmission function

$$P(z) = (1/\Delta\omega) \int\limits_{\omega'}^{\omega''} d\omega \exp\left(-\, k(\omega)\, z\right) . \tag{1}$$

The problem associated with Eq. (1) is apparent, namely, the "palisade" of a great number of spectral lines makes direct (line–by–line) calculation of $\tilde{G}$ so cumbersome that the difficulties are no longer only technical (especially if one deals with "sufficiently large $\Delta\omega$" that is just the case in geophysical applications). The way around this problems by introducing "k–representation" is lively discussed in Refs. 1–15, and the summary of relevant equations is given below for references.

The function (1) is considered to be the Laplace transform for $f(s)$

$$P(z) = \int\limits_0^{\infty} d\, s\, f(s) \exp\left(-\, z\, s\right) ,$$

$$f(s) = (1/2\,\pi\, i) \int\limits_{a-i\,\infty}^{a+i\,\infty} d\, z\, P(z) \exp\left(s\, z\right) , \tag{2}$$

where $a \geq 0$, and further

$$g(s) = \int\limits_0^{s} f(s')\, d\, s' = (1/2\,\pi\, i) \int\limits_{a-i\,\infty}^{a+i\,\infty} d\, z\, (P(z)/z) \exp\left(s\, z\right) \tag{3}$$

with obvious conditions $g(0) = 0$, $g(\infty) = 1$. Now

$$\tilde{G} = (1/\Delta\,\omega) \int\limits_{\omega'}^{\omega''} G(k(\omega))\, d\omega = \int\limits_0^1 G(s(g))\, dg , \tag{4}$$

where $s = s(g)$ is the function inverse to that defined by Eq. (3). The rigorous proof of Eq. (4) is, in fact, the variation on the theme of the Parseval theorem.

Of course, Eq. (4) will greatly simplify the problem only if $k(\omega)$ with its numerous maxima and minima converts to the smooth curve $s(g)$. This hope supported incidentally by numerical simulations is based on a very transparent concept.

The quantity $\exp(-sz)$ in Eq. (2) can be considered as a "spectral transmission with the absorption coefficient s", and $f(s)$ – as the density of probability that $k(\omega) = s$. Furthermore, the first integral in Eq. (2) can be interpreted as the integral from Eq. (1) in which the interval $\Delta\omega$ is at first divided into parts with equal values of k. The quantity (3) finds the meaning of the integral of the probability density and should be a monotonic function with all the consequences ensuing therefrom for $s = s(g)$. (The term "k–distribution" is just introduced from the similar considerations.) In fact, the first problem is reduced exactly to the rigorous proof of the monoton of function (3) and of $s = s(g)$.

Furthermore, the expression (4) may be useful only when function (3) is known; however, the function (1) is already involved in the definition of the last function. The authors of Refs. 1–15 prefer the way when a certain model of the spectrum is chosen, and the corresponding expression for $P(z)$ appears which enters explicitly into Eqs. (2) and (3). To evaluate the model parameters (for example, the average line intensity, the average separation between the lines, etc.), the information on the line characteristics is used and the correction of parameters according to the empirical or line–by–line calculated data is made.

The reasons why such approach to the problem of $g(s)$ should be declared as approximate are quite evident. Firstly, the choice of the model itself is essentially limited by the desire to have the integrals in Eqs. (2) and (3) which can be taken in a closed form. Otherwise, their numerical computation would return the problem, in fact, to the initial Eq. (1). Secondly, the possibility to write down the acceptable expression for $P(z)$ is rigidly regulated by choosing the line shape. Moreover, the description is usually adopted which is valid for the resonance absorption, and the problem of the line periphery, essential for $k(\omega)$ and $P(z)$ (see, for example, Ref. 16) is actually ignored. Thirdly, the transformations (2) and the "inversion" of Eq. (3) have the unpleasant peculiarities of the inverse problems, i.e., they "swing" the errors in $P(z)$. Incidentally, the last circumstance creates a serious obstacle to applying the empirical approximations of the transmission function.

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Then the second problem becomes clear, namely, the direct calculation of $g(s)$ using the spectral line characteristics, avoiding the stage of model construction of the transmission function.

Finally, the third problem consists in choosing formulas for integration of Eq. (4) to minimize the number of terms, for example, in the expression

$$P(z) = \sum_n a_n \exp(-\lambda_n z) , \qquad (5)$$

which is the Dirichlet series with the coefficients a_n and λ_n. As an illustration, the approach of Ref. 17 to the solution of the transfer equation with nonselective characteristics of the aerosol light scattering can be mentioned. Its efficiency is determined, in fact, by the number of terms in series (5).

Of course, all the above–enumerated problems are purely technical, and the systematic and mathematically justified expedient is necessary based on databases of spectroscopic information. Such expedient is presented in Sec. 2, and its additional possibilities in searching the approximate versions of solution of the problem under consideration are shown in Sec. 3.

2. SOME MATHEMATICAL ASPECTS OF *K*–REPRESENTATION

It may appear that the question on relation between $f(s)$ from Eq. (2) and $k(\omega)$ is almost trivial. Indeed, it would suffice to substitute Eq. (1) into the second of Eqs. (2), to interchange the order of integration over ω and z, to change the variable in integration $z = a + i\xi$ and, finding out the representation of the δ–function, to write down

$$f(s) \Rightarrow (1/\Delta\,\omega) \int_{\omega'}^{\omega''} \mathrm{d}\omega\, \delta\,(s - k(\omega)) . \qquad (6)$$

The sign "=" is substituted by "⇒" to underline that the interchange of $\int \mathrm{d}\omega$ and $\int \mathrm{d}z$ was made without proof.

However, the integral (6) will exist only if $k'(\omega) \neq 0$ in the interval $\Delta\omega$, and this condition contradicts physical nature of the problem, i.e., to the "palisade" of spectral lines with numerous maxima and minima. It implies mathematically that the interchange of the order of integration in Eq. (1) and in the second of Eq. (2) is impossible.

Nevertheless, such operation is acceptable after substitution of Eq. (1) into Eq. (3), and the final expression will be

$$g(s) = (1/\Delta\,\omega) \int u(\omega)\, d\omega , \qquad (7)$$

$$k(\omega) \leq s ,\ \omega \in [\omega', \omega''] .$$

In Eq. (7), $u(\omega) = 1$ everywhere except the point $k(\omega) = s$, in which $u = 1/2$. All related to Eqs. (6) and (7) mathematical details are given in Appendix A.

Figure 2 and its consequence Fig. 3 become understandable from expression (7) and from Fig. 1 taken as its illustration. The monoton of Eq. (4) and of $s = s(g)$ which was considered earlier as a plausible hypothesis, appears to be the rigorously proved assertion.

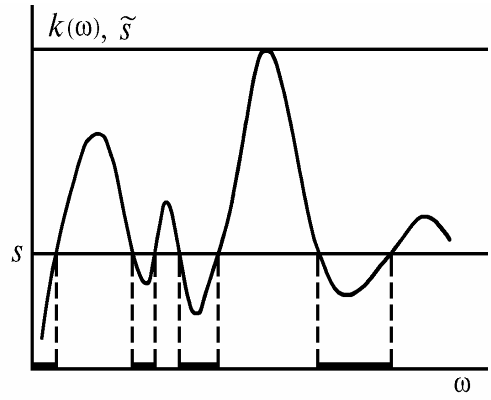

FIG. 1. Function $g(s)$ represents the sum of intervals marked on the abscissa.

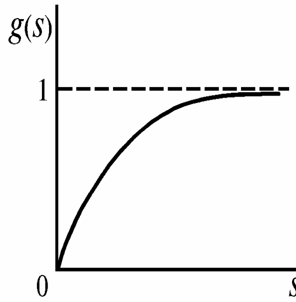

FIG. 2. The "plateau" corresponds to $\tilde{s}$ from Fig. 1.

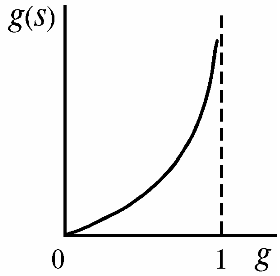

FIG. 3. Function $s(g)$ inverse to $g(s)$, see Fig. 2.

According to formula (7) the function $g(s)$ is calculated immediately through the spectral line characteristics, and the spectral line shape should be naturally used. There is no problem with the overlapping spectra of various gases (with the absorption coefficients k_1, k_2, etc.). Indeed, it is enough to substitute $k_1 + k_2 + \ldots$ for k in Eq. (7). The generalization to the case of nonuniform medium is also evident, namely, k is replaced by the quantity $\int k(\omega, l)\, \mathrm{d}l$, which is the integral of the absorption coefficient over the ray path.

The first and the second problems mentioned in Sec. 1 have been already answered. A small preface should be given before solving the third problem.

The problem on the Dirichlet series of the type of Eq. (5), with the arbitrary function $F(z)$ in the left–hand side was considered in detail in Refs. 18–20. The eigenvalues λ_n should be the simple roots of some suitable integral function $L(\lambda)$ of the complex variable λ; the abscissas a_n are the contour integrals of F and L (see

Appendix B for details). In further calculations the expansion of the exponent appears

$$\exp(-\lambda z) = \sum_n \frac{L(\lambda)}{\lambda - \lambda_n} \frac{1}{L'(\lambda_n)} \exp(-\lambda_n z) . \tag{8}$$

The choice of $L(\lambda)$ is stringently regulated by the convergence condition of the Dirichlet series, by its convergence to its eigenfunction $F(z)$, and by the speed of convergence. Incidentally, these requirements are much simpler if $z > 0$, i.e., the existence of L is beyond question. The problem of construction of the Dirichlet series is solved eventually by the expressions

$$a_n = \int_0^1 \frac{L(s(g))}{s(g) - \lambda_n} \mathrm{d}g \frac{1}{L(\lambda_n)} = \int_0^\infty \frac{L(s) f(s) \mathrm{d}s}{(s - \lambda_n)} \frac{1}{L'(\lambda_n)} , \tag{9}$$

which are obtained as a result of the substitution of Eq. (8) into Eq. (1) (with $\lambda = k(\omega)$) and of the subsequent use of Eq. (4) and then of Eq. (3).

Equation (9) has a quite clear mathematical interpretation, i.e., the polynomials orthogonal with the weight $f(s)$ must be used as L, λ_n are the roots of these polynomials, and Eqs. (9) appear to be the abscissas of the Gaussian quadrature formulas. The meaning of the optimization itself is clarified, namely, among all quadrature formulas the Gaussian formulas are precisely that ones which can be used for calculation of the integrand in the minimum number of points. The problem really returns to function (7), because $f(s) = g'(s)$ by virtue of Eq. (3).

Now the particular, however, pragmatically essential problem should be discussed, connected with the concrete construction of $L(s)$ in Eq. (9). The well–known procedure (see, for example, Ref. 21) implies here the preliminary calculation of μ_n, the "moments" of the function $f(s)$, and the relations (1)–(3) give rise to a chain

$$\mu_n = \int_0^\infty s^n f(s) \,\mathrm{d}s = (\delta_{n0} + n \int_0^\infty (1 - g(s))\, s^{n-1} \,\mathrm{d}s = (-1)^n P^{(n)}(0). \tag{10}$$

Very often in the process of approximating the numerical information on $P(z)$ (empirical one or resulting from line–by–line calculations) the argument of the fitted expression appears to be z to the fractional exponent. It is by no means accidentally. Thus, in the case of the Lorentzian line shape $z \gg 1$ quantity (1) is the function of $\sqrt{z}$, and $1 - P \propto z$, if $z \ll 1$ (see an analysis in Ref. 22). The tendency to describe the behavior, for example, $\ln P$ for all z by this quantity to the power between 1 and 1/2 appears natural.

However, for similar functions the chain (10) does not formally exist, and the mathematical cause of this fact is conditioned by occurring the branch points in the complex plane z that is discussed in Appendix D. This situation can be surely considered as indicative of the very essential "swinging of errors" (its source here is the approximation of $P(z)$), that was already mentioned in Sec. 1 in the preliminary discussion of the problem. It becomes understandable that all the procedure of constructing of μ_n should be fulfilled numerically, using Eqs. (2) and (3), and the corresponding definition from Eq. (10), even if some approximation of $P(z)$ is available. The other way is to find suitable approximation for $f(s)$.

The question under discussion appears to be of principle to some extent, because the branch points and consequently the need of introducing the cut of the plane occur for any radical, among them the radicals appearing almost without exception for models of the absorption bands.

It is worthwhile to note here new pragmatic advantages of the procedure (7), namely, it should radically decrease the volume of calculations necessary for construction of L in Eq. (9), especially in combination with the second expression (10).

3. APPROXIMATE CONSTRUCTION OF THE EXPONENTIAL SERIES FOR FUNCTION (1)

The general properties of the Dirichlet series will enable one to find rather simple (but, of course, approximate) solution of the problem (5) if they are combined with some peculiarities of Eq. (1).

The molecular absorption coefficient $\kappa(\omega) = \sum_j \mathrm{S}_j k_j(\omega, \omega_j)\, S_j \kappa_j(\omega, \omega_j)$ is the sum over the spectral lines with the line centers ω_j, intensities S_j, and line shapes κ_j. Assume, that $\sum_j$ includes the lines of all gases making contributions to the absorption at the frequency ω.

The above–mentioned models of spectra were popular in the atmospheric optics at pre–laser and pre–computer epoch (see, for example, Ref. 22). The computers, as it seemed to be at first, solved the problem by the direct line–by–line calculation. True, their own difficulties emerge, namely, the huge number of lines in $\sum_j$ and, what is the main thing, the problem of the line periphery.

These difficulties can be bypassed, if to use the rather clear expedient of Ref. 23. Let us divide the lines into two groups at the given frequency ω (see Fig. 4) forming κ' and $\tilde{\kappa}$ in κ. The first one involves the lines immediately adjacent to ω (within the interval $\delta\omega$ which is not necessarily coincident with $\Delta\omega$) with the Lorentzian line shape characteristic of the small frequency detunings $|\omega - \omega_j|$ (α_j is the line half–width, and the line center shift is involved in ω_j) $\kappa_j^{(d)} = (\alpha_j/\pi)((\omega - \omega_j)^2 + \alpha_j^2)^{-2}$.

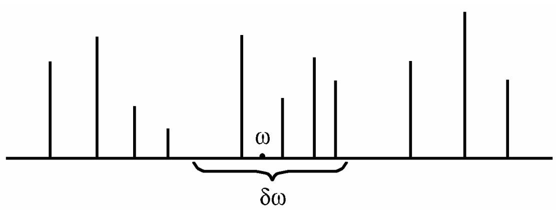

FIG. 4. Spectral lines from the interval δ(ω) forming κ′, the rest ones form $\tilde{\kappa}$.

The second group consists of the distant lines which contribute to the absorption at ω due to their wings. Two essential points should be noted in this connection. First, the parametric description is possible of all similar lines together, that, in fact, eliminates the necessity of summation over a large number of such lines; second, $\bar{\kappa}$ appears to be a smooth function of ω and after substitution $\kappa = \kappa' + \bar{\kappa}$ into Eq. (1), $\exp(-\bar{\kappa}l)$ can be factor out $\int d\omega(\ldots)$, including then $\bar{\kappa}$ into λ_n from Eq. (5).

As it turned out, the realization of this idea ensures the experimental accuracy of calculation (see the examples for atmospheric gases in Refs. 16 and 23). The pragmatic benefit is also evident, i.e., Eq. (1) becomes the problem of evaluating the transmission function of several spectral lines possessing the Lorentzian line shape. It is this function (1) (denoted as P_m with m being equal to the number of lines in the sum κ' and with $\kappa \Rightarrow \kappa'$) which was considered in Refs. 22 and 24 (see, in addition, Ref. 25, where the idea of the approach applied goes back to Ref. 26), and the final expressions are commented below.

Let

$$A = \int_{\omega'}^{\omega''} \left(1 - \exp\left(-\frac{l\,S\,\alpha}{\pi}\frac{1}{(\omega-\omega_0)^2+\alpha^2}\right)\right) d\omega \tag{11}$$

be the absorption function of a single line with intensity S, half–width α, and center ω_0. Then

$$P = 1 - A\ , \quad S = (\beta_2 - \beta_1)\sum_{j=1}^{m} S_j\,\Gamma_j\ ,$$

$$\Gamma_j = \arctan\left((\omega' - \omega_j)/\alpha_j\right) + \arctan\left((\omega'' - \omega_j)/\alpha_j\right)\ ,$$

$$\beta_1 = \arctan((\omega' - \omega_0)/\alpha)\ , \quad \beta_2 = \arctan((\omega'' - \omega_0)/\alpha_j)\ . \tag{12}$$

In sum (12) and expression (7) the absorption lines can belong to different gases, and Eq. (11) is simply generalized to the case of Doppler broadening. Note in addition that Eqs. (11) and (12) ensure the realistic asymptotic behavior of A, namely, the asymptotic case "rather weak absorption".

The quantities α and ω_0 should be considered as parameters, fitted in such a manner that the asymptotic behavior "rather strong absorption" is realized. It is well known[22] that in this version quantity (11) is determined by the interval of integration $(\omega - \omega_j)^2 \gg \alpha^2$, and the same rule is kept for the absorption function with several lines. The evident requirement appears in this case, namely, for ω removed far enough from ω_j

$$S\,\alpha\,/\,(\omega - \omega_0)^{-2} \cong \sum_j S_j\,\alpha_j\,/\,(\omega - \omega_j)^{-2}\ . \tag{13}$$

It is also clear that Eqs. (12) and (13) will give a correct result in the limiting case $m = 1$.

The fact that $\Delta\omega$ and $\delta\omega$ (see Fig. 4) are not necessarily coincident ensures a pragmatic possibility to improve the approximation.

Let us divide the interval $\Delta\omega$ into subintervals $\Delta\omega_j$ in such a manner that only a single line with a center ω_j falls into $\Delta\omega_j$. The transmission function for m lines and for arbitrary $\Delta\omega$ is denoted as $P_m\{\Delta\omega_j\}$. It is obvious that

$$P_m\,\{\Delta\,\omega\} = \sum_{j=1}^{m} P_m\,\{\Delta\,\omega_j\}\,(\Delta\,\omega_j/\Delta\,\omega)\ . \tag{14}$$

Let us apply to $P_m\{\Delta\omega_j\}$ the expedient leading to Eqs. (11) and (12). Now Γ_j from Eq. (12) should be replaced by $\Gamma_{jj'}$ with the index j' numbering the lines and j numbering the subintervals in Eq. (14). Now there is no problem with the choice of ω in Eq. (13).

The formula (14) describes, incidentally, one more correct asymptotic case, i.e., the situation when the line overlapping can be ignored. In this case $\Gamma_{jj'} = \delta_{jj'}$ and Eqs. (11)–(14) convert into the asymptotic sum of the transmission functions of individual lines.

The other important consequence of the analysis performed is the natural definition of the dimensionless "length" z which was introduced still in Eq. (1). It follows from Eq. (11) that it is meaningful to put

$$z = (1/2\,(\beta_2 - \beta_1))\,\alpha\,\pi \sum_{j=1}^{m} S_j\,\Gamma_j \tag{15}$$

with notation from Eq. (12). Of course, after division (14) the corresponding value (15) presents $P_m\{\Delta\omega_j\}$.

When Eq. (11) is represented by the Dirichlet series, Tchebycheff's polynomials should play the role of $L(\lambda)$ (see Appendices B and C). The direct calculations show that the number of terms of series (5) does not exceed five even in the limit of large z. Of course, the values (15) are specific for every summand of Eq. (14), and the total number of summands appears to be large. This problem, in fact, is solved very easily.

Actually, let z_j be the value (15) for jth interval in Eq. (14), and $P_m\{\Delta\omega_j\} = \sum_{n=1}^{N} a_n^{(j)}\exp(-\lambda_n z_j)$ with the known $a_n^{(j)}$, λ_n, and integer N (the last is regulated by a desired accuracy of calculation). Further the quantity $\lambda^{(j)} z_j$, corresponding to $\bar{\kappa}$, is added to $\lambda_n z_j$ (see the discussion of Fig. 4). Equation (15) is introduced for the entire interval and the values $b_j = z_j/z$ are determined. The expansion (8) being applied to $\exp(-z\lambda_r^{(j)})$ with $\lambda_r^{(j)} = b_j(\lambda_n + \lambda^{(j)})$ results in

$$P = \sum_{n=1}^{N} D_n \exp\left(-\lambda_n z\right)\ ,$$

$$D_n = \sum_j \sum_{n=1}^{N} (\Delta\,\omega_j/\Delta\,\omega)\, d_r^{(j)} \frac{L(\lambda_n)}{(\lambda_j^{(j)} - \lambda_n)\,L'(\lambda_n)}\ . \tag{16}$$

The possibility to retain the previous N in Eq. (16) follows simply from numerical estimates.

The numerical analysis of the problem of the expansion of function (11) was performed by Nesmelova, and the peculiarities of the construction of L in Eq. (9) became clear after calculations made by Rodimova. The author expresses them his sincere appreciation.

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APPENDIX A

It follows from Eq. (6) that it is sufficient to know the behavior of the integrand in the vicinity of $\tilde{\omega}$ which is a root of the equation $k(\omega) = s$, i.e., the expression $k(\omega) = s + k'(\tilde{\omega})(\omega - \tilde{\omega}) + (1/2)k''(\tilde{\omega})(\omega\ \tilde{\omega})^2 + \ldots$ can be written. Substituting this expression into the algebraic representation of the δ–function $\delta(x) = (1/\pi) \lim_{\eta\to 0}\eta(x^2 + \eta^2)^{-1}$ and taking into account only first two terms of the expansion at $k(\tilde{\omega}) \neq 0$, we obtain ($\eta\, k(\tilde{\omega}) \Rightarrow \varepsilon$)

$$\delta\,(x - k(\omega)) = \frac{1}{\pi}\lim_{\varepsilon\to 0}\frac{1}{|k(\tilde{\omega})|}\frac{\varepsilon}{(\omega-\tilde{\omega})^2+\varepsilon^2} = \frac{1}{|k(\tilde{\omega})|}\,\mathrm{d}(\omega-\tilde{\omega}).$$

The contribution of these points to Eq. (7) is equal to $(\Delta\omega)^{-1}|k(\tilde{\omega})|^{-1}$.

If however, $k(\omega) = 0$ (this is the case when the straight line $s = \mathrm{const}$ in Fig. 1 is tangent to a maximum or minimum), then the use of the summand $(1/2)k''(\tilde{\omega})(\omega - \tilde{\omega})^2$ in the expansion of $k(\omega)$ will be necessary, and the calculations according to the previous scenarium do not remove η; it remains in the denominator, and the integral (6) goes into infinity.

One more attempt to remove the divergence in Eq. (6) (in a sense of generalized integration) consists in the asymptotic evaluation of integrals

$$(1/2\,\pi\, i)\int_{a-i\infty}^{a+i\infty}\mathrm{d}\,z\,(1/\Delta\omega)\int_{\omega'}^{\omega''}\mathrm{d}\,\omega\,\exp\,(-\,k(\omega)\,z + s\,z)\;.$$

Here the interchange of integrals is necessary to understand the role of points $\tilde{\omega}$.

Now the substitution of the expansion of $k(\omega)$ in the case of $k'(\tilde{\omega}) \neq 0$ returns one to the situation already considered, i.e., after the standard asymptotic integration over ω the quantity $2|\kappa(\tilde{\omega})|z$ appears, and the occurring integral $\int dz$ is equal to 1/2. If $k(\tilde{\omega}) = 0$, then the term $\propto(\omega - \tilde{\omega})^2$ will enter into the asymptotic estimate that leads to the factor $\sim 1/\sqrt{z}$, and the integral $\int dz$ appears to be divergent.

It is well known in the mathematical analysis (see, for example, Ref. 27) that the equality (for a function $\varphi(\omega, z)$)

$$\int_{\omega'}^{\omega''}\mathrm{d}\,\omega\int_{a-i\infty}^{a+i\infty}\mathrm{d}\,z\;\varphi\,(\omega,\,z) = \int_{a-i\infty}^{a+i\infty}\mathrm{d}\,z\int_{\omega'}^{\omega''}\mathrm{d}\,\omega\;\varphi\,(\omega,\,z)$$

exists only in the case of the uniform convergence of the integral with infinite limits in ω, i.e., when

$$\left|\int_{B}^{B'}\mathrm{d}\,z\;\varphi(\omega,\,z)\right| < \varepsilon\;.$$

The last condition is accompanied by the standard comment, namely, for any $\varepsilon > 0$ such B_0 can be found that the inequality written above will be true for all ω, if $B > B' > B_0$.

The substitution of Eq. (1) into the second of Eqs. (2) or into Eq. (3) finds the pragmatic meaning when the transition to $\int d\omega \int dz$ is possible, because only in this case $\int dz$ can be calculated explicity. In the version with Eqs. (1) and (2) the function $\varphi(\omega, z) = \exp z(s - k(\omega))$, and the integral contained in the criterion of the uniform convergence is proportional to

$$(2(s - k(\omega)))^{-1}\,\sin(s - k(\omega))\,(B - B')\;.$$

It is clear that $(B - B')$ can be replaced by infinity, and then the last expression converts into $\delta(s - k(\omega))$ which was studied earlier and which asserts, in fact, that the uniform convergence is absent.

In the case of Eq. (3) the function $\varphi(\omega, z) = (1/z) \times \exp z(s - k(\omega))$, and for sufficiently large B and B' the quantity

$$(B(s - k(\omega)))^{-1}\,\sin(s - k(\omega))\,(B - B')$$

is present in the estimate of the uniform convergence. If $s \neq k(\omega)$, the last expression will vanish at $B \Rightarrow \infty$; if $s = k(\omega)$, the value $(B - B')/B$, independent on ω, will appear, that actually implies the uniform convergence of $\int dz$.

Note, in addition, that after the substitution of Eq. (1) into Eq. (3) and after interchanging the order of integration the well–known integral (see, for example, Ref. 28) occurs

$$\frac{1}{2\pi i}\int_{a-i\infty}^{a+i\infty}\frac{\mathrm{d}\,z}{z}\exp\,z\,(s - k(\omega)) = \begin{cases} 1, & s > k(\omega) \\ (1/2), & s = k(\omega)\,, \\ 0\;, & s < k(\omega) \end{cases}$$

that just leads to Eq. (7).

APPENDIX B

One of the assertions of the Dirichlet theory states that, if $z > 0$, then

$$\frac{1}{2\pi\; ir\,!}\int_{a-i\infty}^{a+i\infty}\mathrm{d}\,z\,\frac{F(z)}{z}\exp\,(s\,z) = \sum_{n=1}^{n'}(s - \lambda_n)^r\,a_n\;,\; a > 0$$

for integer r and $\lambda_{n'} < s < \lambda_{n'+1}$. After the substitution of Eq. (1) for F the calculation of the integral in the last expression repeats literally the derivation of Eq. (7),

$$\frac{1}{\Delta\,\omega}\int_{k(\omega)\,\le\, s} u(\omega)\,(s - k(\omega))^r\,\mathrm{d}\,\omega = \sum_{n=1}^{n'}(s - \lambda_n)\,a_n\;,$$

$s \in [\omega', \omega'']$.

The mathematical interpretation of similar relations is quite obvious, namely, for $g(s)$, the properties of which are demonstrated in Fig. 2, the function $L(\lambda)$ must be padded with zeros in the limited interval dense everywhere, and a sequence is chosen from them of the roots of the polynomials which are orthogonal with the weight $f(s)$.

Let us apply these results to $F(z) = I_n(z)$, the modified Bessel function occurring in Eq. (11) (see, for example, Ref. 22).

To calculate the integral arisen let us use the contour shown in Fig. 5, including the possibility to bypass the point $z = 0$ along the half–circle with the radius ρ. It is clear that for the available integrand the integral over such a contour is equal to zero. For sufficiently large T in the intervals I–II and III–IV the function I_n is replaced by its asymptotic expression $\sim(\xi \pm i\infty)\exp(\pm(\xi + iT))$, and the subsequent modulus evaluation results in

$$\lim_{T\to\infty} \frac{1}{T^{1/2}} \int_0^{a/T} \frac{\mathrm{d}\,y}{(\,y^2 + 1)^{3/4}} = 0\ .$$

The integral under study takes the form

$$\frac{i^{\,n-1}}{2\pi} \int_{-\infty}^{\infty} \frac{\mathrm{d}\,y}{y} J_n(\,y)(\cos sy + i \sin sy) =$$

$$= \begin{cases} 0,\ \ s \geq 1, \\ (-1)^n (1/\pi n) \sin (n \arcsin s),\ s \leq 1,\ r - \text{even}, \\ (-1)^{(n+1)/2} (1/\pi n) \cos (n \arcsin s),\ s \leq 1,\ n - \text{odd}\ , \end{cases}$$

where $z = i\,y$, $I_n(iy) = i^{\,n} J_n(y)$, and J_n is the standard Bessel function. The half–circle is needed only at $n = 0$ and in the case of presence of cos–function in formulas; however, it does not affect the final result.

The last formula is the excellent illustration of the previous general derivation, namely, s changes continuously, and the transition $n \to \infty$ in Eq. (5) implies the transition to the integration. All problems of the Dirichlet series come down to the existence of the integral in the sense of Riemann and the positive answer in the case under consideration is almost obvious.

Thus, let us divide the interval [0, 1] into small parts $\Delta\lambda$ (with the index q) and putting all $\lambda_n = \lambda_q$ in each part, we obtain the expression $\sum\limits_q \exp(-\lambda_q\, z) \sum\limits_{n\in q} a_n$. It is clear that $\sum\limits_{n\in q} a_n = H(\lambda_{q+1}) - H(\lambda_q) \tilde{=} (\partial H/\partial s)\Delta\lambda$, with H being the value of the last integral. It can be seen that the sum over n comes into the integral resulting in the corresponding integral representation for I_n.

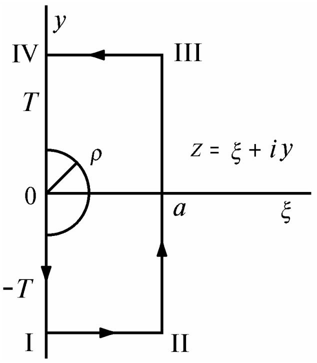

FIG. 5. $T \Rightarrow \infty$ and $\rho \Rightarrow 0$.

The only condition for $L(\lambda)$ implies that it has to have the adequately placed roots. The last expression, in fact, asserts that Tchebycheff's polynomials should be chosen as L (see their properties in Ref. 29, for example). This solves the problem on the choice of L, when the approximation "isolated line" is used in Eq. (1).

APPENDIX C

After simple replacements of variables Eq. (11) will take the form

$$W \equiv \Delta\,\omega\, A = \int_{-\pi}^{\pi} (1 - \exp[-\,z\,(1 + \cos\psi)])\, \frac{\mathrm{d}\,\psi}{1 + \cos\psi}\ ,$$

if the interval $\Delta\omega$ is sufficiently large and, as a consequence, in Eqs. (12) and (15) $\beta_{1,\,2} = \mp(\pi/2)$ are assumed. Of course, the last integral is well–known: $K = 2\pi(I_0(z) + I_1(z))$ with modified Bessel functions.

Choosing Tchebycheff's polynomials as $L(\lambda)$, we can write

$$K = \frac{2\,\pi}{N} \sum_{n=1}^{N} \frac{1 - \exp(-\,z\,(1 + \cos\psi_n))}{1 + \cos\psi_n}$$

with $\psi_n = (2n - 1)/2N$. Consequently, in constructing Eq. (16) $\lambda_n = 1/a_n = 1 + \cos\psi_n$.

APPENDIX D

Let us remind briefly the procedure of the proof of Eq. (10) in accordance with the theory of the Laplace transform.

After substitution of Eq. (2) into the definition of μ_n from Eq. (10), replacing the variable $z = a + iy$ and going to the limit $a \Rightarrow 0$, we obtain

$$\mu_n = \int_{-\infty}^{\infty} \mathrm{d}s\, s^n \int_{-\infty}^{\infty} \mathrm{d}y\, P(i\,y) \exp(i\,y\,s)\ .$$

The fact that the inverse Laplace transform gives $f(s) = 0$ at $s < 0$ has been already used. Therefore, the integration over s is formally performed from $-\infty$. However, the main point here is that $a \Rightarrow 0$ is possible only for the function $P(z)$ regular at the point $z = 0$ that is assured by the initial Eq. (1). The interchange of the order of integration in the last expression is evidently possible; the integral $\int \mathrm{d}s(\ldots)$ results in $i^{-n}\delta^{(n)}(y)$, and the properties of the δ–function enable one to obtain the last expression of the chain (10).

However, when we empirically approximate $P(z)$ by the functions with fraction powers of z, $P(z)$ is no longer regular in the zero point. This point should be removed making the cut of the plane along the negative part of the real axis, and the previous simplifications of μ_n become impossible. It is understandable that the cut of the plane, regardless of the point of its beginning, essentially regulates the analytical properties of $P(z)$ and $f(s)$, and, consequently, the relations between them.

Now some comments should be made about the feasibility to use the approximations $f(s)$ in Eq. (10). Those $f(s)$ which correspond to Eq. (3) and Fig. 2 can be fitted, for example, by the expressions of the type

$$f(s) = (1/\Gamma((\nu + 1)/\gamma))\, s^{\nu} \exp(-\,h\, s^{\nu})$$

with the parameters h, ν, and γ. (The gamma–function appears as a normalization factor, see Eq. (10) for $n = 0$.) Furthermore, Eq. (2) with this $f(s)$ should be written and the parameters should be found using a suitable empirical or model expression for $P(z)$.

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