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New Approach to Estimation of Thermal Broadening of Neutron Resonances

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Abstract. The thermal broadening functions in the Bethe-Placzek approximation, is possible to be present in the form of convolution of one Lorentzian and one Guaussian density. This convolution often named as Voigt-profile or Voigt-function. The computation of this profile is required in several problems arising in a variety of physicochemical subjects, such as nuclear reactors, atmospheric infrared penetrance and several problems of spectroscopy. In this work we suggest using a new formulaes for the calculation of these functions. Our new calculation instruments are representation in the form of finite sums of simple mathematical expressions, based on quadrature formulae, rational approximations and error estimation. They give the good results for the fast calculations, aimed to neutron resonance spectrometry. These approximations can be realized by simple computer codes.

Keywords: Bethe-Placzek approximation, Complex probability function, Voigt-profile.

1 Introduction

The phenomenon of thermal motion of the target atoms respectively nuclei inside a gas or thermal vibration of the atoms respectively nuclei in solid state crystal lattice is well presented by the microscopic cross section of the neutron-nucleus interaction through the effect of thermal broadening. The precise determination of the thermal broadening function and interference term are important for the calculation of the resonance integrals, self-shielding factors. These functions are necessary for corrections of the measurements of the microscopic cross sections with the use of the activation technique [1] and for sample temperature measurement [2]. Moreover these functions are requisite to the description of the distribution of the power in the reactor core and other important applications – numerical simulation of spectral line shapes of typical atmospheric gases [3], analyses of infrared atmospheric measurements [4].

In the recent years the interest to calculation of these functions on the base of new methods and approximations is observed again: [5–9]. These proofs are aimed to several problems connected with fast numerical simulation of line-profiles, where the thermal motion of the molecules or the atoms affect the profile, which are mathematical like to Bethe-Placzek [[10, 11] expression, and to neutron resonance profile – the clear application form of this approximation.

Our finally aim, is fast numerical simulation of neutron resonance profiles in width energy range in resolved resonance region for given nuclides, in order to quality analyses of these nuclides on the base of the known resonance data.

2 Basic Definitions and Aims

Thermal broadening function ψ and interference term χ in the form of Bethe-Placzek approximation for neutron resonance profile usually as follows:

$$\psi(E,\xi) = \frac{\xi}{2\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \frac{e^{-\frac{\xi^2}{4}[D(E)-y]^2}}{1+y^2} dy, \qquad (1)$$

$$\chi(E,\xi) = \frac{\xi}{2\sqrt{\pi}} \int\limits_{-\infty}^{\infty} \frac{e^{-\frac{\xi^2}{4}[D(E)-y]^2}}{1+y^2} y dy \qquad (2)$$

are defined, where the relative resonance distance $D(E)$ is given as

$$D(E) = 2\frac{E-E_\lambda}{\Gamma_\lambda}\ , \qquad (3)$$

E is the current energy (energy of incident neutron) in the vicinity of the resonance energy noted with E_λ, Γ_λ is the full width of the resonance, $\xi = \Gamma_\lambda/\Delta$, where

$$\Delta = \sqrt{\frac{4E_\lambda k_B T}{A}}\ , \qquad (4)$$

k_B is the constant of Boltzmann, T is the temperature of gas, or effectively temperature of solid state lattice, A is the atomic number of the target.

In the vicinity of the resonance energy E_λ, the reaction cross-section with the help of one-level Bright-Wigner formalism and $\psi(E,\xi)$ is given as follows:

$$\sigma_r = \frac{4\pi}{k_\lambda^2} g \frac{\Gamma_{\lambda n}\Gamma_{\lambda r}}{\Gamma_\lambda^2} \sqrt{\frac{E_\lambda}{E}} \psi(E,\xi), \qquad (5)$$

where $\Gamma_{\lambda n}$ is the neutron width, $\Gamma_{\lambda r}$ – the reaction width, $k_\lambda = \sqrt{2m_n E_\lambda/\hbar^2}$ is the wave number of the incident neutron in the resonance, m_n – the mass of the neutron, $g = (2J_\lambda+1)/[2(2I+1)]$, I – the spin of the target nucleus, J_λ – the spin of the compound. The scattering cross-section is given as follows:

$$\sigma_{es} = \sigma_p + \frac{4\pi}{k_\lambda^2} g \Big[\frac{\Gamma_{\lambda n}}{\Gamma_\lambda} \psi(E,\xi) + k_\lambda R \chi(E,\xi) \Big], \qquad (6)$$

where σ_p is the potential cross-section, $R \approx r_0(A^{1/3}+1)$.

The utilization of Bethe-Placzek approximations given by Eq. (5) and Eq. (6) for the thermal broadening instead of exact expression for thermal broadened reaction cross section $\langle\sigma\rangle$ for incident neutron with speed $v = \sqrt{2E/m_n}$ in vicinity of the isolated resonance, with the help of Bright-Wigner one-level formalism, presented as follows:

$$\langle\sigma\rangle = \frac{4\pi}{k_\lambda^2} g \frac{\Gamma_{\lambda n}\Gamma_{\lambda r}}{\Gamma_\lambda^2}$$
$$\times \sqrt{\frac{E_\lambda}{E}} \int_0^\infty \frac{e^{-(v-w)^2/u^2} - e^{-(v+w)^2/u^2}}{1 + [2(\varepsilon(w) - E_\lambda)/\Gamma_\lambda]^2} \frac{w^2 dw}{u v^2 \sqrt{\pi}}, \qquad (7a)$$

or instead of effective broadened cross-section for incoherent Debye solid [12]:

$$\sigma_{\text{eff}}(E) = \sigma_0 \hbar \int_{-\infty}^{\infty} \frac{S(\mathbf{k},\omega)}{1 + [2(E - \hbar\omega - E_\lambda)/\Gamma_\lambda]^2} d\omega \qquad (7b)$$

is justified for majority of applications, at some reservations and elucidations, with the exception of the cases of low energy resonances at very high target temperatures.

For more details about $\langle\sigma\rangle$ given by (7a) see Ref. [13], where it is assumed that the target nuclei have the same velocity distribution as the atoms of an ideal gas, i.e. the Maxwell-Boltzmann distribution, $u^2 = 2k_B T/M_t$, M_t is the mass of target, $\mu = m_n M_t/(m_n + M_t)$ is the reduced mass, $\varepsilon(w) = \mu w^2/2$.

The $S(\mathbf{k},\omega)$ is the scattering function, $\mathbf{k}$ is the wave vector of incident neutron: $\mathbf{k} = \mathbf{p}/\hbar$, hence $E = \mathbf{p}^2/(2m_n) = \hbar\mathbf{k}^2/(2m_n)$, for more details see Ref. [12].

After some simple calculations and rearrangements, the expressions of $\psi(E,\xi)$ and $\chi(E,\xi)$ can be rewritten in the form

$$\frac{\sqrt{\pi}}{\eta}\psi(E,\xi) = \int_{-\infty}^{\infty} \frac{e^{-[x(E)-\eta y]^2}}{1+y^2} dy\,, \qquad (8a)$$

$$\frac{\sqrt{\pi}}{\eta}\chi(E,\xi) = \int_{-\infty}^{\infty} \frac{e^{-[x(E)-\eta y]^2}}{1+y^2} y\,dy\,, \qquad (8b)$$

but now $\eta = \Gamma_\lambda/(2\Delta)$ and $x(E) = (E - E_\lambda)/\Delta$. From Eq. (8a) and Eq. (8b), it follows:

$$\frac{\sqrt{\pi}}{\eta}[\psi(E,\xi) + i\chi(E,\xi)] = J\,, \qquad (9)$$

where

$$J = \int_{-\infty}^{\infty} \frac{e^{-[x(E)-\eta y]^2}}{1+y^2}(1+iy)dy\,.c_3 = a_3 - b_3. \qquad (10)$$

Henceforth we will write x instead of $x(E)$. Further all the presented methods and estimations are aimed to approximately calculation of the integral J, represented by Eq. (10).

3 Basic Mathematical Instruments

After substituting the simple equality,

$$\frac{1+iy}{1+y^2} = \frac{1}{1-iy}\,, \qquad (11)$$

in Eq. (10), we obtain the following representation of J:

$$J = \int_{-\infty}^{\infty} \frac{e^{-(\eta y - x)^2}}{1 - iy} dy\,. \qquad (12)$$

Using the integral equality

$$\frac{1}{1-iy} = \int_0^\infty e^{-u(1-iy)} du\,, \qquad (13)$$

with the aid of Eq. (12), we obtain another representation of J,

$$J = \int_0^\infty \left(\int_{-\infty}^{\infty} e^{-(\eta y - x)^2 + i\frac{u}{\eta}(\eta y - x)} dy \right) e^{i\frac{u}{\eta}(x + i\eta)} du$$
$$= 2\sqrt{\pi} \int_0^\infty e^{-u^2 + 2uif} du \qquad (14)$$

in the form near to Gaussian integral where $f = x + i\eta$. Introducing in Eq. (12) new integration variable, $z = \eta y - x$, we obtain for J representation like to complex probability function [2, 4]

$$J = i \int_{-\infty}^{\infty} \frac{e^{-z^2}}{z+f} dz\,. \qquad (15)$$

The representations given by Eq. (14) and Eq. (15), are our starting points to build the effective approximations of J.

4 The First Approximation

The first approximation, we obtain by using Eq. (15), Eq. (A3) and Eq. (A16)

$$J = i \int_{-\infty}^{\infty} \frac{a(z)}{z+f} dz - i \int_{-\infty}^{\infty} \frac{R(z)}{z+f} dz\,, \qquad (16a)$$

where

$$R(z) = \frac{24}{24 + 24z^2 + 12z^4 + 4z^6 + z^8} - e^{-z^2}\,. \qquad (16b)$$

It satisfies the following: $R(z) = R(-z)$, $R(0) = 0$, $R(\infty) \to 0$; if $z \neq 0$ then $R(z) > 0$, if $|z| \leq 0.4$ then $0 \leq R(z) \leq 10^{-6}$. With the aid of Eq. (B6), we obtain

$$J = -24\pi \sum_{n=1}^{4} \frac{Y_n}{f + L_n} - i \int_{-\infty}^{\infty} \frac{R(z)}{z+f} dz\,. \qquad (17)$$

The approach to approximately calculation of the remainder

$$\int_{-\infty}^{\infty} \frac{R(z)}{z+f} dz\,, \tag{18}$$

we will build on the base of the following integral identity:

$$\int_{-\infty}^{\infty} \frac{R(z)}{z+f} dz = \frac{\pi}{2} \int_{-1}^{1} \frac{t^2(s)+1}{t(s)+f} R(t(s)) ds\,. \tag{19}$$

It is obtained after a new variable $t(s) = \tan(\pi s/2)$, $-1 \le s \le 1$ is introduced in Eq. (18). After substituting in Eq. (19) the following simple equality:

$$\frac{t^2(s)+1}{t(s)+f} = t(s) - f + \frac{1+f^2}{t(s)+f}\,, \tag{20}$$

we obtain

$$\int_{-\infty}^{\infty} \frac{R(z)}{z+f} dz = \frac{\pi}{2}(1+f^2) \int_{-1}^{1} R(t(s)) \frac{ds}{t(s)+f} - \frac{\pi}{2} D f, \tag{21}$$

where $D = \int_{-1}^{1} R(t(s)) ds$. With the aid of Gaussian quadrature of even number of the abscissas

$$\int_{-1}^{+1} h(x)u(x)dx \approx \sum_{n=1}^{N} w_n u(t_n)[h(t_n) + h(-t_n)]\,, \tag{22}$$

where $u(x)$ is an even function, t_n are the abscissas – roots of Legendre's polynomial of grade n, w_n are the weights [14], we obtain

$$\int_{-1}^{1} R(t(s)) \frac{ds}{t(s)+f} \approx f \sum_{n=1}^{N} \frac{g_n}{f^2 - c_n^2}\,, \tag{23}$$

where

$$c_n = \tan(\pi t_n/2)\,, \tag{23a}$$
$$g_n = 2 w_n R(\tan(\pi t_n/2))\,. \tag{23b}$$

Finally for the first approximation, we can write

$$J \approx \frac{\pi i}{2} f \left[D - (1+f^2) \sum_{n=1}^{N} \frac{g_n}{f^2 - c_n^2} \right] - 24\pi \sum_{n=1}^{4} \frac{Y_n}{f + L_n}\,. \tag{24}$$

The L_n are given by Eqs. (A17–A20), Y_n by Eqs. (B7–B10), $D \approx \sum_{n=1}^{N} g_n$. This approximation is without singularities caused by the poles of the type

$$f = -L_n\,. \tag{25}$$

Since, $\eta > 0$, Im $L_n > 0$, hence $f + L_n \neq 0$ always.

From Eq. (9) follows:

$$\psi \approx \frac{\eta}{\sqrt{\pi}} \,\mathrm{Re}\, J, \qquad \chi \approx \frac{\eta}{\sqrt{\pi}} \,\mathrm{Im}\, J. \tag{26}$$

We present in Table 1 calculated 40 decimal logarithms of g_n and same for c_n, the ratios of t_n and w_n, are tacking according to Ref. [14].

Table 1. The decimal logarithms of c_n and g_n calculated according to Eq.(23a) and Eq.(23b) with the aid of the abscissas and the weights of Gaussian quadrature formula

n	$\log_{10}(c_n)$	$-\log_{10}(g_n)$	n	$\log_{10}(c_n)$	$-\log_{10}(g_n)$
1	6.253129	26.272488	21	0.551051	3.191274
2	4.854757	20.312353	22	0.458859	3.187530
3	4.080612	17.020140	23	0.368177	3.248209
4	3.545842	14.747437	24	0.278376	3.366665
5	3.137483	13.013052	25	0.188811	3.537076
6	2.807283	11.611885	26	0.098803	3.765896
7	2.530178	10.437639	27	0.007611	4.015882
8	2.291456	9.428149	28	-0.085595	4.318701
9	2.081739	8.543991	29	-0.181785	4.662734
10	1.894659	7.758640	30	-0.282125	5.049482
11	1.725681	7.053468	31	-0.388067	5.482824
12	1.571454	6.414991	32	-0.501488	5.968697
13	1.429413	5.833233	33	-0.624916	6.517952
14	1.297543	5.300764	34	-0.761910	7.156660
15	1.174222	4.812421	35	-0.917768	7.825293
16	1.058111	4.367954	36	-1.100943	8.926656
17	0.948084	3.977576	37	-1.326274	9.412099
18	0.843174	3.658086	38	-1.623778	9.005226
19	0.742529	3.420650	39	-2.070958	9.067472
20	0.645388	3.266644	40	-3.026938	9.015580

5 The Second Approximation

The second approximation, we obtain by using Eq. (14) rearranged in the form

$$\frac{1}{2i\sqrt{\pi}} \left(J - \sqrt{\pi} \int_{-\infty}^{\infty} e^{-u^2} \cos(2uf) du \right) = \int_{0}^{\infty} e^{-u^2} \sin(2uf) du \tag{27}$$

with the aid of the well-known Euler's formula $e^{iz} = \cos z + i \sin z$. In the integral in the right-hand side of Eq. (27), we introduce a new variable

$$u(y) = \sqrt{-\beta \ln(1 - y^\alpha)}\,, \tag{28}$$

where $0 \le y \le 1$, $\alpha > 1$, $\beta > 1$. With the aid of Gaussian integral

$$\int_{-\infty}^{\infty} e^{-y^2} \cos(ay) dy = \sqrt{\pi} e^{-a^2/4}, \tag{29a}$$

and first derivative of $u(y)$

$$\frac{d}{dy} u(y) = \frac{\alpha\sqrt{\beta}}{2\sqrt{-\ln(1-y^\alpha)}} \frac{y^{\alpha-1}}{1-y^\alpha}, \tag{29b}$$

we obtain

$$\frac{J - \pi e^{-f^2}}{i\sqrt{\beta}\pi\alpha} = \int_{0}^{1} \frac{\sin\left(2f\sqrt{-\beta\ln(1-y^\alpha)}\right)}{\sqrt{-\ln(1-y^\alpha)}} \times y^{\alpha-1} (1-y^\alpha)^{\beta-1} dy\,. \tag{30}$$

With the help of Simpson's integration rule [15,16], we obtain that

$$\frac{J-\pi e^{-f^2}}{i\sqrt{\beta\pi}\alpha}=S(N)-R\,. \tag{31}$$

The sum $S(N)$ is given as follows:

$$S\,(N)=\frac{1}{3N}\sum_{m=1}^{N-1}(2P_m+Q_m), \tag{32}$$

where

$$P_m=\left[1-\left(\frac{m-1/2}{N}\right)^{\alpha}\right]^{\beta-1}\left(\frac{m-1/2}{N}\right)^{\alpha-1}\times F\left(\frac{m-1/2}{N}\right), \tag{33}$$

$$Q_m=\left[1-\left(\frac{m}{N}\right)^{\alpha}\right]^{\beta-1}\left(\frac{m}{N}\right)^{\alpha-1}F\left(\frac{m}{N}\right), \tag{34}$$

$$F(y)=\frac{\sin\left(2f\sqrt{-\beta\ln(1-y^{\alpha})}\right)}{\sqrt{-\ln(1-y^{\alpha})}}\,. \tag{35}$$

The remainder R is given as follows:

$$R=\frac{D(y_0)}{2880N^4}\,, \tag{36}$$

where

$$D(y_0)=\frac{d^4}{dy^4}\left[F(y)y^{\alpha-1}(1-y^{\alpha})^{\beta-1}\right]\Big|_{y=y_0} \tag{37}$$

with a domain for y_0 given as follows: $0\le y_0\le 1$. For $\alpha>5$, and $\beta>6$, the 4th derivative in the right-hand side of Eq. (37) is a regular function of y in the domain $0\le y\le 1$, see Appendix C. In this case the remainder R decreases, if N increases. From Eq. (9) and Eq. (31) follows:

$$\psi\approx\eta\,\mathrm{Re}(\sqrt{\pi}e^{-f^2}+i\alpha\sqrt{\beta}S(N))\,, \tag{38}$$

$$\chi\approx\eta\,\mathrm{Im}(\sqrt{\pi}e^{-f^2}+i\alpha\sqrt{\beta}S(N))\,. \tag{39}$$

With the help of Eq. (31) and Eq. (36), carefully can be written chain of approximate equalities,

$$r(N_1)=r(N_2)=\cdots=r(N_k)=\cdots=r(N_{j-1})=r(N_j), \tag{40}$$

at some reservations, for definiteness: N_k, as $k=1,2,\ldots,j-1,j$, are ordered in this way: $N_{k+1}>N_k$, and $r(N_k)$ is given as

$$r(N_k)=\left[\frac{J-\pi e^{-f^2}}{i\alpha\sqrt{\beta\pi}}-S(N_k)\right]N_k^4\,. \tag{41}$$

These relations are good starting points to Richardson's extrapolation $r(N_k)=r(N_{k+1})$, that is

$$J=\pi e^{-f^2}+i\alpha\sqrt{\beta\pi}\Big\{S(N_k)+\frac{1}{1-\rho^4}[S(N_{k+1})-S(N_k)]\Big\}, \tag{42}$$

where $\rho=N_k/N_{k+1}$.

6 Conclusions

We present an estimation obtained by rational approximation of the exponential function: $\exp(-z^2)$ and high-accuracy computation of the remainder, this is the first approximation. In the principle the function $\exp(-z^2)$ can be expanded in the form like to Eq. (A16) with the help of $K=5$, 6, 7,..., etc. in Eq. (A2), on the base of the procedure described in Appendix A. However in this case the roots of one algebraic equation like to Eq. (A4) must be calculated numerically, it is very difficult problem. Nevertheless it is possible to obtain in this way an accurate expression for the integral J given by Eq. (15) like to Eq. (16a) and Eq. (24) with $K>4$ and numerically estimated remainder at $N<40$ according to Eq. (23). This approach can be an alternative to other methods existing in the literature.

The second approximation is obtained by numerical integration rule for the integral representation in the right hand side of Eq. (30). In contrast to Gaussian quadrature formula, the integration rule of Simpson is free from the external separately estimated parameters like to abscissas or weights. They are very simple calculated in Simpson's rule. This make more flexible formulae given by Eq. (32), moreover lighten the calculations with Eq. (42).

The present approximations of the thermal broadening are expressed in terms of elementary functions and elementary function of an elementary function, that allow the calculation of their values in an efficient and fast manner. Thanks to simple representations, the proposed thermal broadening functions approximations are efficient for implementation in the rapid algorithms.

APPENDIX A

On the base of the well-known exponential expansion

$$e^z=1+\sum_{n=1}^{\infty}\frac{z^n}{n!}\,, \tag{A1}$$

we introduce the following approximation:

$$e^{-z^2}=\frac{1}{e^{z^2}}\approx\frac{1}{1+\sum_{n=1}^{K}z^{2n}/n!}=a(z)\,. \tag{A2}$$

If $K=4$ then,

$$a(z)=\frac{24}{24+24z^2+12z^4+4z^6+z^8}\,. \tag{A3}$$

With the aid of the binominal relation: $(z^2+1)^4=z^8+4z^6+6z^4+4z^2+1$, after simple calculations and rearrangements, we obtain

$$24+24z^2+12z^4+4z^6+z^8=9+8(z^2+1)+6(z^2+1)^2+(z^2+1)^4\,. \tag{A4}$$

Finally we have

$$a(z)=\frac{24}{9+8y+6y^2+y^4}\,, \tag{A5}$$

where $y=z^2+1$.

In order to present the 4th grade equation: $y^4 + 6y^2 + 8y + 9 = 0$, in the form of the product of the two square equations, as follows:

$$y^4 + 6y^2 + 8y + 9 = (y^2 + py + q)(y^2 - py + 9/q) = 0\,, \quad \text{(A6a)}$$

we compare the coefficients before y and y^2 in the left hand side of Eq. (A6a) with the coefficients before y and y^2 in the right hand side of the algebraic product,

$$(y^2 + py + q)(y^2 - py + 9/q) = y^4 + (q - p^2 + 9/q)y^2 + p(9/q - q)y + 9\,. \quad \text{(A6b)}$$

Finally we obtain the following equations for the unknown parameters p and q:

$$q - p^2 + 9/q = 6\,, \quad \text{(A7)}$$

$$p(9/q - q) = 8\,. \quad \text{(A8)}$$

In the principle, some simple manipulations over Eq. (A7) and Eq. (A8) lead to two the separated equations, as follows: the first cubic equation: $x^3 - 3x/16 - 1/64 = 0$, where $x = 1/p^2$, and the second equation: $q = 3 + p^2/2 - 4/p$. According to the well-known formula for the solution of the cubic equation, we have

$$x = s_1^{1/3} + s_2^{1/3}\,, \quad \text{(A9a)}$$

where s_1, s_2 are the solutions of the quadratic equation $s^2 - 2^{-6}s + 2^{-12} = 0$. Finally we obtain, $s_{1,2} = 2^{-6}e^{\pm i\pi/3}$, therefore $x = (1/2)\cos(\pi/9)$,

$$p = 1/\sqrt{x} = 1.45892\,, \quad \text{(A9b)}$$

$$q = 3 + p^2/2 - 4/p = 1.32248\,. \quad \text{(A9c)}$$

The roots of the square equation $y^2 + py + q = 0$ are

$$r_1 = -0.729462 + i0.889025\,, \quad \text{(A10a)}$$

$$r_2 = r_1^*\,. \quad \text{(A10b)}$$

Same for $y^2 - py + 9/q = 0$,

$$r_3 = 0.729462 + i2.504653\,, \quad \text{(A10c)}$$

$$r_4 = r_3^*\,. \quad \text{(A10d)}$$

On the base of the obtained roots, the expression in right hand side of Eq. (A5) can be written in the form of the following algebraic expansion:

$$\frac{1}{9 + 8(z^2+1) + 6(z^2+1)^2 + (z^2+1)^4} = \sum_{n=1}^{4} \frac{C_n}{z^2 + 1 - r_n}\,, \quad \text{(A11)}$$

where

$$C_1 = \frac{1}{(r_1 - r_2)(r_1 - r_3)(r_1 - r_4)}\,, \quad \text{(A12)}$$

$$C_2 = \frac{1}{(r_2 - r_1)(r_2 - r_3)(r_2 - r_4)}\,, \quad \text{(A13)}$$

$$C_3 = \frac{1}{(r_3 - r_1)(r_3 - r_2)(r_3 - r_4)}\,, \quad \text{(A14)}$$

$$C_4 = \frac{1}{(r_4 - r_1)(r_4 - r_2)(r_4 - r_3)}\,. \quad \text{(A15)}$$

Finally

$$a(z) = 12\sum_{n=1}^{4} \frac{C_n}{L_n}\Big(\frac{1}{z - L_n} - \frac{1}{z + L_n}\Big)\,, \quad \text{(A16)}$$

here $L_n = i\sqrt{1 - r_n}$, given as follows:

$$L_1 = 0.32796 + i1.35537\,, \quad \text{(A17)}$$

$$L_2 = -L_1^*\,, \quad \text{(A18)}$$

$$L_3 = 1.06035 + i1.18105\,, \quad \text{(A19)}$$

$$L_4 = -L_3^*\,. \quad \text{(A20)}$$

APPENDIX B

If $C_1 = R_1 + iI_1$ and $C_2 = R_2 + iI_2$ are complex numbers, $I_1 \neq 0$, $I_2 \neq 0$, then

$$\int_{-\infty}^{\infty} \frac{dz}{(z + C_1)(z + C_2)} = \frac{1}{C_2 - C_1}\lim_{g\to\infty}\Big(\ln\frac{C_2 - g}{C_2 + g} + \ln\frac{C_1 + g}{C_1 - g}\Big) = \frac{\pi i}{C_2 - C_1}s(I_1, I_2)\,, \quad \text{(B1)}$$

where

$$s(I_1, I_2) = \frac{I_2}{|I_2|} - \frac{I_1}{|I_1|}\,. \quad \text{(B2)}$$

With the help of Eq. (A16) we can write

$$\int_{-\infty}^{\infty} \frac{a(z)}{z + f}dz = 12\sum_{n=1}^{4}\frac{C_n}{L_n}\int_{-\infty}^{\infty}\Big(\frac{1}{z - L_n} - \frac{1}{z + L_n}\Big)\frac{dz}{z + f}\,, \quad \text{(B3)}$$

From Eq. (B1) follows:

$$\int_{-\infty}^{\infty} \frac{a(z)}{z + f}dz = 12\pi i\sum_{n=1}^{4}\frac{C_n}{L_n}\Big[\frac{s(\mathrm{Im}\,(-L_n), \eta)}{f + L_n} - \frac{s(\mathrm{Im}\,(+L_n), \eta)}{f - L_n}\Big]\,, \quad \text{(B4)}$$

where

$$s(\mathrm{Im}\,(\mp L_n), \eta) = 1 - \frac{\mathrm{Im}\,(\mp L_n)}{|\mathrm{Im}\,(\mp L_n)|}\,, \quad \text{(B5)}$$

because $\eta > 0$. From Eqs. (A17–A20), follows: $\mathrm{Im}\,L_n > 0$, for $n = 1, 2, 3, 4$, therefore,

$$\int_{-\infty}^{\infty} \frac{a(z)}{z + f}dz = 24\pi i\sum_{n=1}^{4}\frac{Y_n}{f + L_n}\,, \quad \text{(B6)}$$

where $Y_n = C_n/L_n$, after calculation, we have

$$Y_1 = -0.0423372 - i0.0268911\,, \quad \text{(B7)}$$

$$Y_2 = +0.0423372 - i0.0268911\,, \quad \text{(B8)}$$

$$Y_3 = -0.0046415 + i0.0149365\,, \quad \text{(B9)}$$

$$Y_4 = +0.0046415 + i0.0149365\,. \quad \text{(B10)}$$

APPENDIX C

Using the expansion

$$\frac{\sin(z)}{z} = 1 + \sum_{m=1}^{\infty} \frac{(-1)^m z^{2m}}{(2m+1)!} \tag{C1}$$

and expression for $F(y)$ presented by Eq. (35)

$$F(y) = \frac{\sin\left(2\sqrt{\beta} f \sqrt{-\ln(1-y^\alpha)}\right)}{\sqrt{-\ln(1-y^\alpha)}}, \tag{C2}$$

we obtain the following:

$$F(y) = 2f\sqrt{\beta} \sum_{m=0}^{\infty} \frac{(-1)^m}{(2m+1)!} \left(2f\sqrt{\beta}\right)^{2m} \times \left[\ln \frac{1}{1-y^\alpha}\right]^m. \tag{C3}$$

With the aid of Eq. (D7), we obtain

$$\left(2f\sqrt{\beta}\right)^{2m} \left[\ln \frac{1}{1-y^\alpha}\right]^m = \frac{\gamma}{2\pi} \int_0^1 t^{\gamma-1} dt \int_0^{2\pi} \left(2fe^{-i\frac{s}{2}} \sqrt{\beta\gamma \ln \frac{1}{t}}\right)^{2m} \times (1-y^\alpha)^{-\exp(is)} ds. \tag{C4}$$

After substitute Eq. (C4) in Eq. (C3), we have

$$F(y) = \frac{\sqrt{\gamma}}{2\pi} \int_0^1 \frac{t^{\gamma-1} dt}{\sqrt{-\ln t}} \int_0^{2\pi} \Psi(s,t)(1-y^\alpha)^{-\exp(is)} ds, \tag{C5}$$

where

$$\Psi(s,t) = e^{is/2} \sin\left(2\sqrt{\beta\gamma} f e^{-is/2} \sqrt{-\ln t}\right). \tag{C6}$$

From Eq. (37) follows:

$$D(y) = \frac{\sqrt{\gamma}}{2\pi} \int_0^1 \frac{t^{\gamma-1} dt}{\sqrt{-\ln t}} \times \int_0^{2\pi} \Psi(s,t) \frac{d^4}{dy^4} [y^{\alpha-1}(1-y^\alpha)^{g(s)}] ds. \tag{C7}$$

where $g(s) = \beta - e^{is} - 1$. By simple calculations, we obtain

$$\frac{d^4}{dy^4} \left[y^{\alpha-1}(1-y^\alpha)^{g(s)}\right] = y^{\alpha-1} j_4 + w_4 (1-y^\alpha)^{g(s)} + 4(w_1 j_3 + w_3 j_1) + 6 w_2 j_2, \tag{C8}$$

where

$$w_n = \frac{d^n}{dy^n} y^{\alpha-1} = y^{\alpha-(n+1)} \prod_{q=1}^{n} (\alpha - q), \tag{C9}$$

$$j_n = \frac{d^n}{dy^n} (1-y^\alpha)^{g(s)}. \tag{C10}$$

For j_1, j_2, j_3, j_4, we obtain

$$j_1 = -\alpha g(s)(1-y^\alpha)^{g(s)-1} y^{\alpha-1}, \tag{C11}$$

$$j_2 = \Phi_1 \varphi_2 + \Phi_2 \varphi_1^2, \tag{C12}$$

$$j_3 = \Phi_1 \varphi_3 + 3\Phi_2 \varphi_1 \varphi_2 + \Phi_3 \varphi_1^3, \tag{C13}$$

$$j_4 = \Phi_1 \varphi_4 + \Phi_2 (4\varphi_1 \varphi_3 + 3\varphi_2^2) + 6\Phi_3 \varphi_1^2 \varphi_2 + \Phi_4 \varphi_1^4, \tag{C14}$$

where

$$\Phi_n = \frac{d^n}{dh^n} h^{g(s)}\Big|_{h=1-y^\alpha} = (1-y^\alpha)^{g(s)-n} \prod_{q=1}^{n} [g(s) - q + 1], \tag{C15}$$

$$\varphi_n = -\frac{d^n}{dy^n} y^\alpha = -y^{\alpha-n} \prod_{q=1}^{n} (\alpha - q + 1). \tag{C16}$$

Therefore, if $\alpha > 5$ and $\beta - \cos(s) - 1 > 4$ in the domain: $0 \le s \le 2\pi$, i.e. $\beta > 6$, then $|\text{Re}\, D(y)| < \infty$, $|\text{Im}\, D(y)| < \infty$ in the domain $0 \le y \le 1$, moreover $D(0) = D(1) = 0$.

APPENDIX D

With the help of the well-known exponential expansion

$$\exp(z) = 1 + \sum_{n=1}^{\infty} \frac{z^n}{n!}, \tag{D1}$$

we obtain the flowing:

$$\exp(ze^{iy}) = 1 + \sum_{n=1}^{\infty} \frac{z^n e^{iny}}{n!}. \tag{D2}$$

If $|k| = 0, 1, 2, 3, \ldots$, then

$$\frac{1}{2\pi} \int_0^{2\pi} e^{iky} dy = \begin{cases} 1 & \text{if} \quad k = 0 \\ 0 & \text{if} \quad |k| \neq 0 \end{cases}. \tag{D3}$$

From Eq. (D2) and Eq. (D3) follows:

$$\frac{z^m}{m!} = \frac{1}{2\pi} \int_0^{2\pi} e^{-imy} \exp(ze^{iy}) dy. \tag{D4}$$

By using integral representation

$$m! = \gamma \int_0^1 \left(\gamma \ln \frac{1}{t}\right)^m t^{\gamma-1} dt, \qquad \gamma > 1, \tag{D5}$$

in Eq. (D4), we obtain that

$$z^m = \frac{\gamma}{2\pi} \int_0^1 t^{\gamma-1} dt \int_0^{2\pi} \left(e^{-i\frac{y}{2}} \sqrt{\gamma \ln \frac{1}{t}}\right)^{2m} \exp(ze^{iy}) dy. \tag{D6}$$

If $z = \ln h$, then

$$(\ln h)^m = \frac{\gamma}{2\pi} \int_0^1 t^{\gamma-1} dt \int_0^{2\pi} \left(e^{-i\frac{y}{2}} \sqrt{\gamma \ln \frac{1}{t}}\right)^{2m} h^{\exp(iy)} dy. \tag{D7}$$

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