

INVERSION OF THE CORRELATION FUNCTION OF PARTICLE SHADOWS: ANALYTIC TECHNIQUES

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Analytic solutions to the inverse problem of retrieval of the particle size distribution function from measurements of the correlation function of their shadows have been found. Such solutions are of interest for the development of the method of diagnosing coarsely dispersed media from multiply scattered radiation treated in the small-angle approximation.

One of the widespread techniques used for solving the equation of radiative transfer (ERT) in the small-angle (SA) approximation is based on approximating the integral term of ERT by the operator of convolution.^{1,2} It is then possible to obtain a simple analytic solution to ERT, which is described, among the other optical characteristics of a medium, by the Fourier transform of the small-angle scattering phase function. In the approximation of the Fraunhofer diffraction, this transform represents the correlation function of particle shadows (CFPS), whose form depends on the disperse composition of a medium.³ Using dimensionless coordinates, the CFPS of a system of spherical scatterers $\varphi(\xi)$ is expressed as⁴

$$\varphi(\xi) = \int_{\xi}^1 G(\xi/\eta) f(\eta) d\eta, \quad (1)$$

where $\xi \in [0, 1]$, the function $f(\eta)$ has the meaning of the normalized distribution function of particles over their relative size $\eta = r/R$ (R is the maximum radius of scatterers), and the kernel of transformation (1) is

$$G(t) = \begin{cases} \frac{2}{\pi} [\arccos t - t\sqrt{1-t^2}], & t \leq 1, \\ 0, & t > 1. \end{cases} \quad (2)$$

If data are available on the dependence $\varphi(\xi)$, one may set the inverse problem of retrieving the disperse composition of a medium from integral equation (1). That information is, in its turn, contained in such fundamental solutions of the small-angle ERT, as function of coherence, intensity of a plane wave, optical transfer function, and point spread function, that are controlled by the form of CFPS $\varphi(\xi)$ and may be used to retrieve it. Such problems were considered in detail in Refs. 4–6. A finite difference regularizing algorithm for numerical inversion of CFPS $\varphi(\xi)$, described by Eq. (1), was reported in Ref. 4. The form of kernel $G(t)$ given by Eq. (2) permits various functional transformations of Eq. (1) to be applied that lead to well-known types of integral equations and make it possible to obtain an analytic solution. The present article considers techniques for analytic inversion of CFPS $\varphi(\xi)$ given by Eq. (1).

1. DIFFERENTIATION TECHNIQUE

On differentiating Eq. (1) with respect to ξ , we obtain

$$\int_{\xi}^1 f(\eta) \eta^{-1} \sqrt{1 - (\xi/\eta)^2} d\eta = -\frac{\pi}{4} \frac{d\varphi(\xi)}{d\xi}. \quad (3)$$

If we consider the zero-order Hankel transform of the function $\varphi(\xi)$

$$x(\omega) = \int_0^1 \xi J_0(\omega\xi) \varphi(\xi) d\xi, \quad (4)$$

which defines the scattering phase function, then the derivative $\varphi'(\xi)$ entering in the right-hand side of Eq. (3) may be represented as the first-order Hankel transform of the function $\omega x(\omega)$

$$\frac{d\varphi(\xi)}{d\xi} = \int_0^{\infty} \omega^2 J_1(\omega\xi) x(\omega) d\omega. \quad (5)$$

Let us substitute variables in Eq. (3)

$$x = \eta^2, \quad y = \xi^2. \quad (6)$$

Then the integral in Eq. (3) may be represented as a cross-correlation

$$\int_y^1 f_1(x) \sqrt{x-y} dx = \varphi_1(y) \quad (7)$$

of an unknown function

$$f(x) = x^{-3/2} f(\sqrt{x}) \quad (8)$$

with the kernel

$$g(x) = \sqrt{x} U(x), \quad U(x) = \begin{cases} 1, & x \geq 0, \\ 0, & x < 0, \end{cases} \quad (9)$$

where

$$\varphi_1(y) = - \frac{\pi}{2} \left. \frac{d\varphi(\xi)}{d\xi} \right|_{\xi = \sqrt{y}} \quad (10)$$

Accounting for the relation between the correlation and the convolution of two functions derived in Ref. 7, we may apply the technique of the Fourier transform to solve integral equation (7). Efficient numerical techniques are available for solving the equations of the convolution type, based on taking the discrete Fourier transform.⁸

Differentiating Eq. (3) once more, we arrive at the Abel–type equation

$$\int_{\xi}^1 \frac{f(\eta) d\eta}{\eta^2 \sqrt{\eta^2 - \xi^2}} = \frac{\pi}{4} \frac{d^2 \varphi(\xi)}{\xi d\xi^2} \quad (11)$$

Its solution may be written in the form

$$f(\eta) = - \frac{\eta^3}{2} \int_{\eta}^1 \frac{d}{d\xi} \left[\frac{1}{\xi} \frac{d^2 \varphi(\xi)}{d\xi^2} \right] \frac{d\xi}{\sqrt{\xi^2 - \eta^2}} \quad (12)$$

Many physical problems are reduced to the Abel–type equation. Much attention has been paid to the development of numerical algorithms and to their solution. A review of the existing inversion techniques and algorithms for inversion of the Abel equation may be found, e.g., in Ref. 9.

A disadvantage of the above–considered technique is the need to differentiate the measured correlation function of particle shadows $\varphi(\xi)$, which is always known within the limits of error, so the resulting problem is ill–posed and calls for regularization. Below we consider those approaches that obviate the need for differentiating measurable functions.

2. TECHNIQUE OF FOURIER TRANSFORM

If we represent Eq. (7) in the form of a convolution $f_1 \times g_1 = \varphi_1$, where $g_1(x) = g(-x)$, Eq. (7) acquires the following form in the frequency domain:

$$F_1(\omega) G_1(\omega) = \Phi_1(\omega), \quad (13)$$

where $F_1(\omega)$ and $\Phi_1(\omega)$ are the Fourier transforms of the functions $f_1(x)$ and $\varphi_1(x)$, $G_1(\omega) = G_1(-\omega)$, and

$$G_1(\omega) = (\sqrt{\pi} / 2) (1 / |\omega|^{3/2}) \exp(\pm i 3\pi / 4) \quad (14)$$

is the Fourier transform of the function $g(x) = \sqrt{x} U(x)$ (see Ref. 7). The minus sign is chosen in case $\omega > 0$, and the plus – in case $\omega < 0$. It may be demonstrated that the inverse kernel for Eq. (13) is determined by the function

$$\frac{1}{G_1(\omega)} = - \frac{4}{\pi} (i \omega)^3 G_1(\omega), \quad (15)$$

and the solution of Eq. (7) in the frequency domain has the form

$$F_1(\omega) = - \frac{4}{\pi} (i \omega)^3 G_1(\omega) \Phi_1(\omega). \quad (16)$$

We represent the right–hand side of Eq. (16) as a product

$$F_1(\omega) = - \frac{4}{\pi} [(i \omega) G_1(\omega)] [(i \omega)^2 \Phi_1(\omega)]. \quad (17)$$

A function of the form

$$g_2(x) = - \frac{U(-x)}{2 \sqrt{-x}} \quad (18)$$

corresponds to the Fourier transform of $[(i \omega) G_1(\omega)]$. The inverse Fourier transform given by Eq. (17) then yields a solution of Eq. (7) in the form of a cross–correlation for the functions $(1/\sqrt{x}) U(x)$ and $\varphi''(y)$

$$f_1(x) = \frac{2}{\pi} \int_x^1 \frac{\varphi''_1(y) dy}{\sqrt{y-x}} \quad (19)$$

Making the inverse change of variables in Eq. (19) $\eta = \sqrt{x}$, $\xi = \sqrt{y}$, we arrive at a solution which corresponds exactly to the solution of Eq. (12) obtained by inversion of the Abel equation (11).

Another form of the solution may be obtained if we represent Eq. (16) in the form

$$F_1(\omega) = - \frac{4}{\pi} [(i \omega)^3 G_1(\omega)] \Phi_1(\omega). \quad (20)$$

Similarly to the above–considered case, we may demonstrate that the solution $f_1(x)$, whose Fourier transform is determined by relation (20), is a cross–correlation between the third derivative of the function $\sqrt{x} U(x)$ and the function $\varphi_1(y)$, that is,

$$f_1(x) = \frac{4}{\pi} \int_0^{1-x} \frac{d^3}{dy^3} [\sqrt{y} U(y)] \varphi_1(y+x) dy \quad (21)$$

If we express the function $\varphi_1(y)$ given by Eq. (10) in terms of the scattering phase function $x(\omega)$ using relation (5), then we obviate the need for differentiation of $\varphi(\xi)$ while retrieving the disperse composition of a medium from expression (21).

3. TECHNIQUE OF FUNCTIONAL TRANSFORMATIONS

As has already been mentioned above, the disadvantage of the solution in the form of formula (12) is the need for differentiation of the CFPS $\varphi(\xi)$. One possible way to circumvent this difficulty consists in using the Hankel transform $x(\omega)$ of the function $\varphi(\xi)$ given by Eq. (4).

Expressing the correlation function $\varphi(\xi)$ and its derivatives in terms of the Hankel transform of the scattering phase function $x(\omega)$ given by Eq. (4) and using recursion formulae for the Bessel functions,¹⁰ we obtain the following integral representation of the differential term in expression (12):

$$Q(\xi) \equiv \frac{d}{d\xi} \left[\frac{1}{\xi} \frac{d^2 \varphi(\xi)}{d\xi^2} \right] = \int_0^{\infty} K(\xi, \omega) x(\omega) d\omega, \quad (22)$$

in which the transformation kernel $K(\xi, \omega)$ has the form

$$K(\xi, \omega) = \frac{\omega^4}{\xi} J_1(\xi \omega) + 2 \frac{\omega^2}{\xi^2} J_0(\xi \omega) - 3 \frac{\omega^2}{\xi^3} J_1(\xi \omega). \quad (23)$$

As a result, we obtain our solution in the form

$$f(\eta) = -\frac{\eta^3}{2} \int_{\eta}^1 \frac{Q(\xi) d\xi}{\sqrt{\xi^2 - \eta^2}}. \tag{24}$$

Thus the procedure of constructing the solution of Eq. (11) consists in successive application of the Hankel transform given by Eq. (4) to the correlation function $\varphi(\xi)$ and of the integral transformations given by Eqs. (22) and (24); as a result, we find the particle size distribution function $f(\eta)$ without differentiating $\varphi(\xi)$. A disadvantage of this approach is large volume of calculations of the above integrals.

4. TRANSFORMATION TO THE EQUATION OF CONVOLUTION WITHOUT DIFFERENTIATING THE RIGHT-HAND SIDE

The dependence of the kernel of Eq. (1) on the ratio of the arguments ξ/η makes it possible to proceed to the equation of convolution by changing the variables

$$\eta = \eta_0 e^{-\alpha x}, \quad \xi = \xi_0 e^{-\alpha y}. \tag{25}$$

Let us assume, for definiteness, $\xi_0 = \eta_0 = 1$ and choose $\alpha > 0$. The kernel $K(\xi, \omega) = G\{\exp[-\alpha(y-x)]\}$ will then depend on the difference between the new variables. Substituting Eq. (25) into Eq. (1), we obtain the equation of convolution

$$\int_0^y Q(y-x) v(x) dx = u(y), \quad 0 \leq y < \infty, \tag{26}$$

for the function $v(x) = \eta f(\eta)$, where $\eta = \exp(-\alpha x)$, with its kernel $Q(x) = \alpha G \exp(-\alpha x)$ and its right-hand side $u(y) = \varphi(\exp(-\alpha y))$. Unfortunately, the function $Q(x)$ is not absolutely integrable in the interval $[0, \infty)$, so the technique of Fourier transform cannot be applied to solve Eq. (26).

Therefore, we modify Eq. (26) by multiplying its left- and right-hand sides by $\xi = \exp(-\alpha y)$. As a result, we obtain another integral equation of convolution type

$$\int_0^y Q(y-x) \exp(-\alpha(y-x)) v_1(x) dx = u_1(y) \tag{27}$$

for the function $v_1(x) = \eta^2 f(\eta)$, where $\eta = \exp(-\alpha x)$, with its kernel $Q_1(x) = Q(x) \exp(-\alpha x)$ and its right-hand side $u_1(y) = u(y) \exp(-\alpha y)$. The integral

$$\int_0^{\infty} Q_1(x) dx = \int_0^1 G(t) dt = \frac{2}{3\pi} < \infty \tag{28}$$

converges, so we take the Fourier transform to invert Eq. (27).

Similar reasoning may be applied to solve Eq. (3). By substituting variables (25), Eq. (3) may be transformed to the form

$$\int_0^y Q_2(y-x) v(x) dx = u_2(y), \quad 0 \leq y < \infty, \tag{29}$$

in which the unknown function $v(x) = \eta f(\eta)$ is the same as in Eq. (26), the kernel is

$$Q_2(x) = \alpha(1 - \exp(-2\alpha x))^{1/2} \exp(-\alpha x), \tag{30}$$

and the right-hand side $u_2(y)$ is related to the right-hand side of Eq. (26) by the expression

$$u_2(y) = -\frac{\pi}{4} \xi \frac{d\varphi(\xi)}{d\xi} = \frac{\pi}{4} \frac{d u(y)}{\alpha dy}. \tag{31}$$

The function $Q_2(x)$ is absolutely integrable in the interval $[0, \infty)$, and its Fourier transform has the form

$$S(\omega) = \frac{\sqrt{\pi}}{4} \frac{\Gamma[(\alpha + i\omega)/2\alpha]}{\Gamma[(4\alpha + i\omega)/2\alpha]}. \tag{32}$$

If we introduce designations $V(\omega)$ and $U(\omega)$ for the Fourier transforms of the functions $v(x)$ and $u(y)$, respectively, the solution of Eq. (29) in the frequency domain will be given by the formula

$$V(\omega) = \frac{\sqrt{\pi}}{\alpha} (i\omega) \frac{\Gamma[(4\alpha + i\omega)/2\alpha]}{\Gamma[(\alpha + i\omega)/2\alpha]} U(\omega). \tag{33}$$

5. COSINE AND SINE FOURIER TRANSFORMS: THE SOLUTION FOR MOMENTS

We start from Eq. (3), which assumes the form

$$\int_{\xi}^1 \frac{f(\eta)}{\eta^2} \sqrt{\eta^2 - \xi^2} d\eta = -\frac{\pi}{4} \frac{d\varphi(\xi)}{d\xi}. \tag{34}$$

We multiply both sides of Eq. (34) by $\cos(\xi\omega)$ and integrate the result over ξ in the limits from 0 to 1. Changing the order of integration in the left-hand side of Eq. (34) and calculating the internal integral, we then obtain the following equation:

$$\int_0^1 \frac{f(\eta)}{\eta\omega} J_1(\eta\omega) d\eta = -\frac{1}{2} \int_0^1 \frac{d\varphi(\xi)}{d\xi} \cos(\omega\xi) d\xi. \tag{35}$$

To avoid differentiating of the correlation function of particle shadows $\varphi(\xi)$, we take the integral in the right-hand side of Eq. (35) by parts. This yields the function

$$\Gamma(\omega) = \left[1 - \omega \int_0^1 \varphi(\xi) \sin(\omega\xi) d\xi \right] / 2, \tag{36}$$

which defines the first-order Hankel transform of the function $f(\eta)/\eta^2$

$$\int_0^1 \frac{f(\eta)}{\eta^2} J_1(\eta\omega) \eta d\eta = \omega \Gamma(\omega). \tag{37}$$

The inverse transform given by Eq. (37) yields the sought-for distribution

$$f(\eta) = \eta^2 \int_0^{\infty} \Gamma(\omega) J_1(\eta\omega) \omega^2 d\omega. \quad (38)$$

To invert integral equation (34) by this technique, we take the sine Fourier transform of the correlation function $\varphi(\xi)$ and then proceed to the function $\Gamma(\omega)$ given by Eq. (36). The sought-for distribution $f(\eta)$ is then found in the form of the Hankel transform of the function $\omega \Gamma(\omega)$, defined by Eq. (38). The technique described above needs no calculation of the derivative $d\varphi(\xi)/d\xi$. Efficient algorithms are available for calculating the sine Fourier transform and the Hankel transform.

Equation (37) permits simple expressions for moments of the particle size distribution function $f(\eta)$ to be derived. To this end, we expand the Bessel function $J_1(\eta\omega)$ in the integrand of expression (37) and the function $\sin(\omega\xi)$ in the integrand of Eq. (36) in power series. By simple transformations, expression (37) acquires the form

$$\sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa} m_{2\kappa}^f}{2^{2\kappa} \kappa! (\kappa+1)!} \omega^{2\kappa} = \sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa} m_{2\kappa-1}^{\varphi}}{(2\kappa-1)!} \omega^{2\kappa}, \quad (39)$$

where

$$m_{2\kappa}^f = \int_0^1 f(\eta) \eta^{2\kappa} d\eta, \quad \kappa = 1, 2, \dots \quad (40)$$

are the even moments of the particle size distribution functions $f(\eta)$ and

$$m_{2\kappa-1}^{\varphi} = \int_0^1 \varphi(\xi) \xi^{2\kappa-1} d\xi, \quad \kappa = 1, 2, \dots \quad (41)$$

are the odd moments of the correlation function of particle shadows $\varphi(\xi)$.

Equating the coefficients for identical powers of ω in relation (39), we obtain expressions for the even moments of the function $f(\eta)$

$$m_{2\kappa}^f = c_{2\kappa} m_{2\kappa-1}^{\varphi}, \quad \kappa = 1, 2, \dots, \quad (42)$$

where

$$c_{2\kappa} = \frac{2^{2\kappa} \kappa! (\kappa+1)!}{(2\kappa-1)!}. \quad (43)$$

Thus we arrive at the general formulae expressing the 2κ th moments of the sought-for solution $f(\eta)$ in terms of the $(2\kappa-1)$ th moments of the correlation function of shadows $\varphi(\xi)$.

Formulae for the odd moments of the distribution function $f(\eta)$ may be obtained similarly, starting from the sine Fourier transform of the integral equation (34), with subsequent expansion of the cosine Fourier transform of CFPS $\varphi(\xi)$ in a power series. It results in the following relations between the $(2\kappa+1)$ th moment of the particle size

distribution function $f(\eta)$ and the 2κ th moment of the correlation function of particle shadows $\varphi(\xi)$:

$$m_{2\kappa+1}^f = c_{2\kappa+1} m_{2\kappa}^{\varphi}, \quad \kappa = 0, 1, 2, \dots, \quad (44)$$

where

$$c_{2\kappa+1} = \frac{\pi (2\kappa+1)! (2\kappa+3)!}{4 (2\kappa)!}. \quad (45)$$

By combining formulae (42) and (44) we may state that an arbitrary moment m_{κ}^f of the sought-for distribution $f(\eta)$ is expressed in terms of the $(\kappa-1)$ th moment of the correlation function of shadows

$$m_{\kappa}^f = c_{\kappa} m_{\kappa-1}^{\varphi}, \quad \kappa = 1, 2, \dots, \quad (46)$$

where the coefficients c_{κ} are found from formulae (43) and (45).

When solving many applied problems, it may appear quite sufficient to have the first moments of the retrieved distribution $f(\eta)$. If we restrict our consideration to a prescribed model of the distribution function $f(\eta)$ with some unknown parameters, these parameters may be related to the moments of the distribution. For example, for widespread lognormal distribution model

$$f(\eta) = \frac{1}{\eta\sigma\sqrt{2\pi}} \exp\left\{-\frac{(\ln\eta - m)^2}{2\sigma^2}\right\}, \quad (47)$$

its parameters m and σ^2 are related to the first two moments m_1 and m_2 of the distribution $f(\eta)$ by the following expressions:

$$m = \ln\{m_1^2 / \sqrt{m_2}\}, \quad \sigma^2 = \ln[m_2 / m_1^2]. \quad (48)$$

CONCLUSION

The diverse analytic solutions obtained for inverting the CFPS open venues for developing numerical algorithms to retrieve the particle size distribution function. Such algorithms would include standard routines for experimental data processing (such as numerical differentiation, Fourier and Hankel transforms, etc.). Their efficiency would depend on the rate of respective mathematical transformations, on the accuracy of the initial data, on the stability of such algorithms with respect to errors in the initial data, etc. This calls for further dedicated studies.

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