DETERMINATION OF AEROSOL MICROSTRUCTURE FROM PARTICLE SHADOW CORRELATION FUNCTION BY THE METHOD OF THE FOURIER–BESSEL SERIES EXPANSION

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A numerical algorithm is considered for inverting the particle shadow correlation function based on the Hankel transformation and the Fourier–Bessel series expansion of the particle size distribution function. The stability of the inverse problem solution is studied based on an analysis of its conditionality and results of numerical experiments. The algorithm is applicable to solving the problems of aerosol microstructure diagnostics for single and multiple scattering in the small-angle approximation.

The problem of inverting the shadow correlation function (SCF) of particles[1–3] holds a central position in the problem of optical microstructure diagnostics of a coarse–dispersed medium taking into account the multiple scattering. The SCF of particles is unambiguously connected with spatial–angular characteristics of the multiply scattered radiation that can be used for its finding. The dependence of SCF of a polydispersed ensemble of spherical scatterers $\varphi(\xi)$ on the microstructure of a medium is described by the expression

$$\varphi(\xi) = \int\limits_{\xi}^{1} G(\xi/\eta)\, f(\eta)\, d\eta, \qquad (1)$$

where $\xi \in [0, 1]$. The transformation (1) is written in the dimensionless coordinates. Its kernel has the form

$$G(t) = \begin{cases} \frac{2}{\pi}\left[\arccos t - t\sqrt{1-t^2}\,\right], & t \le 1, \\ 0, & t > 1, \end{cases} \qquad (2)$$

and the function $f(\eta)$ has the meaning of the normalized density of particle distribution over size of their geometric cross section.

A technique for solving integral equation (1) using the finite–difference regularizing algorithm was described in Ref. 1. Problems of reconstructing the microstructure of a dispersed medium $f(\eta)$ were considered in Ref. 4 on the basis of analytical transformation of SCF $\varphi(\xi)$.

This paper considers a "hybrid" algorithm for reconstructing the function $f(\eta)$ from Eq. (1). This algorithm includes the integral transformation of SCF $\varphi(\xi)$ and inversion of the matrix equation for determining the coefficients of the Fourier–Bessel series expansion of the function $f(\eta)$.

Using the zero–order Hankel transformation of SCF $\varphi(\xi)$

$$x(\omega) = \int\limits_{0}^{1} \xi\, J_0(\omega\xi)\, \varphi(\xi)\, d\xi, \qquad (3)$$

transition from integral equation (1) to the equation

$$2\int\limits_{0}^{1} J_1^2(\omega\eta/2)\, f(\eta)\, d\eta = H(\omega), \qquad (4)$$

with the right–hand side $H(\omega) = \omega^2 x(\omega)$, is made at the first stage of solving the inverse problem. Let us represent the function $\eta f(\eta)$ in the form of expansion in terms of the complete system of functions $\{J_0(\alpha_i\,\eta)\}$, orthogonal in the interval (0, 1) with weight η:

$$\eta\, f(\eta) = \sum_{i=1}^{\infty} b_i\, J_0(\alpha_i\, \eta), \qquad 0 < \eta < 1\,. \qquad (5)$$

Here α_i are the zeros of the Bessel function $J_0(x)$: $J_0(\alpha_i) = 0$, $i = 1, 2, \dots$.

To determine the coefficients b_i, let us substitute series (5) into Eq. (4). As a result, we obtain the following equation:

$$\sum_{i=1}^{\infty} A_i(\omega)\, b_i = H(\omega) \qquad (6)$$

in unknowns b_i ($i = 1, 2, \dots$) with the coefficients

$$A_i(\omega) = 2\int\limits_{0}^{1} J_0(\alpha_i\, \eta)\, J_1^2(\omega\eta/2)\, \frac{d\eta}{\eta}\,. \qquad (7)$$

The integrand in Eq. (7) decreases quickly as η increases. This makes it possible to replace the finite upper limit of integration in Eq. (7) by infinite one without great loss in accuracy. Then the coefficients $A_i(\omega)$ take a very simple form

$$A_i(\omega) = G(\alpha_i/\omega)\,, \qquad (8)$$

where the function $G(t)$ is determined by Eq. (2). It follows from the properties of the function $G(t)$ that $G(\alpha_i/\omega) = 0$ for $\omega \le \alpha_i$. This makes it possible to select such readings ω_j that the matrix $A_i(\omega_j)$ takes the triangle

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form, and the solution of Eq. (6) becomes trivial. It is necessary to select the readings ω_j from the condition

$$\alpha_j < \omega_j \le \alpha_{j+1}, \qquad j = 1, 2, \dots . \qquad (9)$$

The function $G(t)$ decreases monotonically, its range of variation $1 \ge G(t) \ge 0$ for $t \in [0, 1]$, so the diagonal elements of the matrix $A_i(\omega_j)$ reach their maxima at

$$\omega_j = \alpha_{j+1}, \qquad j = 1, 2, \dots . \qquad (10)$$

With such a selection of the readings ω_j, Eq. (6) transforms to the infinite system of linear equations

$$\sum_{i=1}^{\infty} A_{ji}\, b_i = H_j, \qquad j = 1, 2, \dots \qquad (11)$$

with the lower triangle matrix whose elements are $A_{ji} = G(\alpha_i/\alpha_{j+1})$, $j = 1, 2, \dots,$ $i = 1, 2, \dots, j$, and the right–hand side $H_j = \alpha_{j+1}^2\, x(\alpha_{j+1})$, $j = 1, 2, \dots$, where α_j are the roots of the equation $J_0(z) = 0$.

An arbitrary finite number n of the coefficients $b_i (i = 1, \dots, n)$ of series (6) is determined from the first n equations of system (11). Stability of this system can be characterized by the conditional number $P_n = \max|\lambda_i|/\min|\lambda_i|$, where λ_i are the eigenvalues of the matrix A. Since the matrix A is the lower triangle, its eigenvalues coincide with the diagonal elements, $\lambda_i = G(\alpha_i/\alpha_{i+1})$. The ratios of successive zeros of the Bessel function (α_i/α_{i+1}) form monotonically increasing sequence. So, due to the monotonic character of the function $G(t)$, the expression for the conditional number has the form

$$P_n = \frac{G(\alpha_1/\alpha_2)}{G(\alpha_n/\alpha_{n+1})} . \qquad (12)$$

The results of calculation of the conditional numbers P_n by Eq. (12) are given in Table I for successive values of n.

TABLE I.

n	5	6	7	8	9	10	15	20
P_n	5.1	6.7	8.2	11	12	13	26	33

It follows from Table I that the conditional numbers P_n keep their low values, and the solution of system (11) is stable when the problem dimensionality n is finite and falls within the limits that satisfy the needs of practical calculations.

The solution of system (11) is found by the recursion formulas

$$b_1 = \frac{H_1}{A_{11}}, \qquad b_i = \frac{H_i - \sum_{j=1}^{i-1} A_{ij}\, b_j}{A_{ii}}, \qquad i = 2, 3, \dots . \qquad (13)$$

Substituting the so–determined coefficients b_i into series (5), we obtain the sought–after distribution $f(\eta)$.

Summation of series (5) is unstable towards errors in setting the coefficients b_i, if the error in reconstructing the function $f(\eta)$ is estimated in uniform metric. Stable techniques for summation of the Fourier series on the basis of the conception of regularization were described in Ref. 5. In the simplest case, the limited number of terms in expansion (5) consistent with the errors in determining the coefficients b_i from the system of equations (11) serves this purpose.

It should be noted that analogous procedure for reconstructing the distribution $f(\eta)$ can be constructed based on expansion in terms of the other orthogonal systems of basis functions that are obtained from the system $\{J_0(\alpha_i\eta)\}$ in which α_i are replaced by β_i, the zeros of the Bessel function $J_1(x)$, or by γ_i, the roots of the equation

$$q\, J_0(x) - x\, J_1(x) = 0 . \qquad (14)$$

Here, q is an arbitrary real constant (Dini series[6]).

Let us consider for illustration an example of inversion of the correlation function $\varphi(\xi)$ by the Fourier–Bessel series expansion in numerical experiment. In Fig. 1, the discrepancy $\varepsilon_{\varphi}^{(n)} = > \varphi_n - \varphi_\delta > / > \varphi_\delta >$ (curve *1*) and the error $\varepsilon_f^{(n)} = > f_n - f_T > / > f_T >$ in reconstructing the distribution $f(\eta)$ (curve *2*) are shown as functions of the number of terms in series expansion (5) for a 10% relative error δ in the initial data $\varphi(\xi)$. The model distribution $f_T(\eta)$ is shown in Fig. 2 (curve *1*). It is seen from Fig. 1 (curve *1*) that the satisfactory accuracy of reconstruction of the unimodal distribution $f(\eta)$ is already reached with five terms of the series ($\varepsilon_f^{(5)} = 0.14$). In this case, the discrepancy $\varepsilon_\varphi^{(5)}$ is equal to 0.078. The minimal error in reconstructing $f(\eta)$ is equal to 6.1% and is reached for $n = 11$. With further increase in the number of terms of series expansion (5), summation becomes unstable and leads to a sharp increase of the error $\varepsilon_f^{(n)}$. The fact that when n varies within the limits $3 \le n \le 12$, the discrepancy $\varepsilon_\varphi^{(n)}$ varies insignificantly and does not exceed the error of the initial data ($\varepsilon_\varphi^{(n)} < 10\%$) has engaged our attention. An example of distribution $f(\eta)$ reconstructed for $n = 11$ and a 10% relative error in setting the function $\varphi(\xi)$ is shown in Fig. 2 (curve *2*).

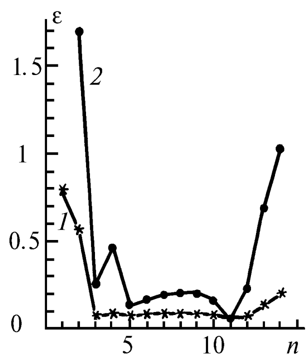

FIG. 1. Relative discrepancy $\varepsilon_\varphi^{(n)}$ (curve 1) and error $\varepsilon_f^{(n)}$ (curve 2) in reconstructing the distribution $f(\eta)$ as functions of the number n of the terms of the Fourier–Bessel series expansion in model experiment with a 10% relative error in the initial data.

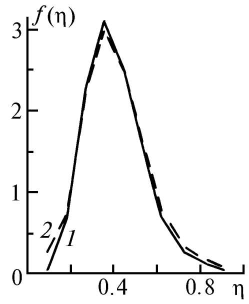

FIG. 2. Example of reconstructing $f(\eta)$ in numerical experiment using the Fourier–Bessel series expansion for a 10% relative error in the initial data: model (1) and result of inverting $\varphi(\xi)$ (2), $n = 11$.

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