SENSITIVITY OF THE POLYDISPERSE INDICATRIX TO THE SHAPE OF THE DISTRIBUTION CURVE

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Abstract

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SENSITIVITY OF THE POLYDISPERSE INDICATRIX TO THE SHAPE OF THE DISTRIBUTION CURVE

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1. The light-scattering indicatrix of a polydisperse colloidal system is determined by the relation

$$\bar{I}(\beta) = \int_0^\infty I(\beta, a) f(a)\, da. \quad (1)$$

Here $\bar{I}(\beta)$ is the polydisperse indicatrix; $I(\beta, a)$ is the scattering indicatrix of an individual particle of radius a; $f(a)$ is the distribution curve; β is the scattering angle.

Formula (1) gives the possibility, in principle, of determining $f(a)$ from the known $I(\beta, a)$ and $\bar{I}(\beta)$, if one inverts the integral equation (1). This equation is a Fredholm equation of the first kind and, generally speaking, as is known, it can determine not the point values of the function $f(a)$, but its mean values along small intervals of the abscissa axis ([1]). For some simple kernels—individual indicatrices $I(\beta, a)$—equation (1) can be inverted exactly, and then we find not averages over small intervals, but the exact values of the function $f(a)$ ([2]). Physically there is no difference between these two cases, since the mean values of $f(a)$ will be close to the exact ones when the subdivision is sufficiently dense. In practice, however, from the computational point of view, the difference here is very great, since in the absence of an exact formula for inverting (1) the problem reduces to solving a system of linear algebraic equations with a large number of unknowns, which is a very laborious operation. For a large class of problems in the optics of turbid media, reduction of the Fredholm integral equation (1) to a system of linear algebraic equations is necessary, since the function $I(\beta, a)$ is usually specified in the form of tables of indicatrices. In this connection an important question arises concerning the well-posedness of the resulting system.

2. The right-hand sides of our system represent the result of an experiment, and therefore they always contain some error. This error, of course, will pass into the final answer. The principal question here is whether the error in the values of the roots of the system of algebraic equations will

be of approximately the same order as the measurement error, or significantly larger. Very often it turns out that the system under consideration is "ill-posed," i.e., small fluctuations in the right-hand sides of the equations will correspond to large fluctuations in the values of the roots of our linear system, and a solution that is quite exact from the mathematical point of view will have no physical meaning because the right-hand sides of the equations are known only with limited accuracy. If one uses an analogy from radio engineering, one should say that our system is noise-unstable: a weak noise at the input is transformed by it into a large signal at the output. In the theory of linear equations such a system is called ill-conditioned. It can be shown that the degree of conditioning of a system is determined by the ratio $\lambda_{\max}/\lambda_{\min}$, where $\lambda_{\max}$ and $\lambda_{\min}$ are, respectively, the maximum and minimum

eigenvalues of the system matrix (the noise amplification coefficient is equal to $\sqrt{\lambda_{\max}/\lambda_{\min}}$). In a poorly conditioned system this ratio is large (of the order 10^3–10^4). A system for which this ratio exceeds 10^4 is not suitable for solving the problem posed.

3. In constructing our system of linear equations we can use scattering indicatrices in different ranges of scattering angles. Naturally, in doing so we must strive to choose indicatrices in that region of angles β where the system is best conditioned; in this case the limited accuracy of the experiment will have the least effect on the result. Thus there arises the important problem of investigating the conditioning of systems of algebraic equations that appear when different portions of the scattering indicatrix are used in the inverse problem of scattering theory. This is a matter of determining the optimal portion of the indicatrix which it is expedient to use in determining $f(a)$. Of course, the answer will depend substantially on those values of a at which $f(a)$ differs appreciably from zero.

4. Let us consider, for example, an aerosol whose microstructure is described by the gamma distribution

$$f(a) = Aa^{\mu} \exp(-\gamma a). \tag{2}$$

Passing to the normalized curve in relative units $a/\bar{a} = \tau$ ($\bar{a}$ is the mean value of a), we obtain

$$f(a) = \left\{ N \frac{(\mu+1)^{\mu+1}}{\mu!} \tau^{\mu} \exp[-(\mu+1)\tau] \right. \tag{3}$$

Formula (3) describes a single-peaked distribution with width

$$\Delta\tau = 2.48/\sqrt{\mu}. \tag{4}$$

The only parameter characterizing the shape of the curve here is μ.

Let us now investigate in what region of scattering angles β the polydisperse indicatrix with distribution (2) is most sensitive to the shape of the distribution curve, i.e., to the parameter μ. In the analysis we use the polydisperse indicatrix corresponding to curve (2) for the case of "soft" particles ([3]). The polydisperse indicatrix $\bar{I}$ is written as follows:

$$I = I_{\text{rel}}(\bar{a})\,\varphi_\mu(u). \tag{5}$$

Here

$$I_{\text{rel}}(\bar{a}) = I_0|\alpha|^2 \frac{128}{9}\frac{\pi^6}{\lambda^4}(1+\cos^2\beta)\bar{a}^6,$$

$$\varphi_\mu(u) = \frac{288}{(\mu+1)^6 u^6}\left\{1 - s^{(\mu+1)}F + \frac{u^2}{4}(\mu+1)(\mu+2)\right\},$$

$$u = \frac{2m}{\gamma} = \frac{2\bar{q}}{\mu+1}, \qquad m = \frac{q}{a} = \frac{4\pi}{\lambda}\sin\frac{\beta}{2}, \tag{6}$$

$$s = (1+u^2)^{-1/2}, \qquad r = \operatorname{arc\,tg} u,$$

$$F = \cos(\mu+1)r + us(\mu+1)\sin(\mu+2)r - \frac{\mu+1}{4}u^2 s^2(\mu+2)\cos(\mu+3)r.$$

Taking the mean particle radius $\bar{a}$ and the number of particles per unit volume as given, we find

$$\frac{d\bar{I}}{d\mu} = I_{\text{rel}}(\bar{a})\frac{d\varphi_\mu}{d\mu} I_{\text{rel}}(\bar{a})F(u,\mu), \tag{7}$$

where

$$F(u,\mu) = -\frac{1}{\mu+1}\left\{6\varphi_\mu(u) + u\frac{\partial\psi}{\partial u}\bigg|_{\mu=\text{const}}\right\} + \frac{288}{(\mu+1)^6u^6}\left\{\frac{u^2}{4}(2\mu+3) - s^{(\mu+1)}F\ln s - s^{(\mu+1)}\frac{\partial F}{\partial\mu}\right\}.$$

The curves $F(u,\mu)$, plotted as a function of the scattering angle β, are shown in Fig. 1. It is seen that the sensitivity of $\bar{I}$ to the form of $f(a)$ (i.e., to μ) increases sharply in the region of small β.

Fig. 1 and Fig. 2

Figure 1: Fig. 1 and Fig. 2

Fig. 1. $\mu = 8$. 1–$\overline{a} = 0.1\,\mu$;
2–$\overline{a} = 0.2\,\mu$

Fig. 2. $\overline{a} = 0.1\,\mu$

5. As another case, let us consider an aerosol with a microstructure of the form

$$f(a) = \frac{A}{a^n}, \qquad a \geq a_{\min};$$

$$f(a) = 0, \qquad 0 < a < a_{\min}. \tag{8}$$

For $n = 4$ we arrive at the Junge distribution.

The polydisperse indicatrices for "soft" particles will now be

$$n = 4, \qquad \overline{I} = I_{\text{rel}}(\overline{a})\,\varphi_2(u), \tag{9}$$

where

$$u = \frac{8\pi}{3\lambda}\,\overline{a}\sin\frac{\beta}{2},$$

$$\varphi_2(u) = \frac{32}{81}\frac{1}{u^6}\{1 - \cos 2u + 3u^2 + \pi u^3 - u^2\cos 2u - 2u\sin 2u - 2u^3\sin 2u\};$$

$$n = 5, \qquad \overline{I} = I_{\text{rel}}(\overline{a})\,\varphi_3(u), \tag{10}$$

where

$$u = \frac{6\pi}{\lambda}\,\overline{a}\sin\frac{\beta}{2},$$

$$\varphi_3(u) = \frac{3^8}{4^3}\frac{1}{u^6}\left\{-\frac{u\sin u}{2} - \frac{\cos u}{2} + \frac{u^2}{4} + \frac{1}{2}\right\};$$

$$n = 6, \qquad \overline{I} = I_{\text{rel}}(\overline{a})\,\varphi_4(u), \tag{11}$$

where

$$u = \frac{32}{5}\frac{\pi}{\lambda}\,\bar{a}\sin\frac{\beta}{2},$$

$$\varphi_4(u) = \frac{3^2 \cdot 2^{18}}{5^6}\,\frac{1}{u^6}\left\{\frac{1}{96}\left[2\left(-24 + 2u^2 - u^4\cos u - 2u(24+u^2)\sin u - 2u^5\sin u + \pi u^5\right)\right] + \frac{1}{2} + \frac{5}{24}u^2\right\}.$$

For the case of the distribution (8), the system of linear equations will have the best conditioning where the indicatrix $\bar{I}(\beta)$ has the greatest rate of change with respect to β. The curve of variation of $d\bar{I}/d\beta$, plotted as a function of β for $n = 4$, $\bar{a} = 0.1\mu$, is given in Fig. 2. It shows that the sensitivity of the indicatrix here, just as in the case of the gamma distribution, increases in the region of small β.

6. The typical examples considered above show that, in order to solve the inverse problem, detailed tables of scattering indicatrices in the region of small angles are necessary. The compilation of such tables appears to us to be one of the important tasks of the optics of turbid media.

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Note: Figure translations are in progress. See original paper for figures.