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Abstract

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INVERSION OF THE INDICATRIX FOR "SOFT" PARTICLES

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1. Let us consider the problem of determining the particle spectrum of a disperse system from data on the scattering indicatrix. In the case of "dilute" systems, when one may restrict oneself to the study of single scattering, the matter reduces to the inversion of a Fredholm integral equation of the first kind

$$\overline{J}(\beta) = \int_0^\infty J(\beta, r) f^*(r)\, dr. \tag{1}$$

Here $f^*(r)$ is the size-distribution curve of the particles; $J(\beta, r)$ is the indicatrix of light scattering by an individual particle of radius r (β is the scattering angle), known from the theory of light scattering (^{1}); $\overline{J}(\beta)$ is the polydisperse indicatrix, determined experimentally. Our problem is to indicate a method for calculating the unknown distribution function $f^*(r)$ from $J(\beta, r)$ and $\overline{J}(\beta)$.

For a system consisting of arbitrary particles, the kernel of the integral equation $J(\beta, r)$ (the monodisperse indicatrix) is usually given in tabular form. In this case one should study various numerical methods for solving such equations. These methods are based on the idea of constructing stable solutions that are insensitive to measurement errors contained in $\overline{J}(\beta)$, and to inversion errors. The main point here is a successful choice of a system of orthogonal functions in which the sought function $f^*(r)$ is to be expanded (^{2}). It is essential that this system contain, as initial terms, functions close to $f^*(r)$. This can always be done, since the approximate form of the distribution function is usually known.

2. There is, however, one important special case when the monodisperse scattering indicatrix $J(\beta, r)$ is expressed by a simple analytic formula. This concerns particles whose optical properties differ little from the properties of the surrounding medium, for which the quantities

$$\rho(m-1) < 1, \qquad \rho = \frac{2\pi r}{\lambda}, \qquad \alpha = \frac{3}{4\pi}\frac{m^2-1}{m^2+1} < 1 \tag{2}$$

(for more detail see (^{1})). Here λ is the wavelength, and m is the refractive index. For "soft" particles the formula (^{1}) is valid

$$J(\beta, r) = I_0 \psi(\beta) \frac{(\sin q - q\cos q)^2}{q^2} r^2, \qquad \psi(\beta) = 2\pi^2 |\alpha|^2 \frac{1+\cos^2\beta}{(1-\cos\beta)^2},$$

$$q = 2\rho \sin\frac{\beta}{2}. \tag{3}$$

Let us pass to dimensionless variables

$$a = \frac{r}{r_0}, \qquad f(a) = f^*(r) r_0^4, \tag{4}$$

where r_0 is the linear scale of the problem, and put

$$b = \sin\frac{\beta}{2}, \qquad \gamma = \frac{4\pi r_0}{\lambda}, \qquad x = 2\gamma b. \tag{5}$$

The integral equation (1) in dimensionless variables takes the form

$$g(\gamma b) = \int_0^\infty K(q) m(a)\, da, \qquad q = \gamma a b, \tag{6}$$

where

$$g(\gamma b) = \frac{r}{\psi(\beta)} \frac{\overline{J}(\beta)}{I_0}, \qquad K(q) = \frac{(\sin q - q\cos q)^2}{q^2}, \qquad m(a) = a^2 f(a). \tag{7}$$

3. Let $L(p)$ and $G(p)$ denote the Mellin transforms, with respect to the variable b, of the functions $K(\gamma b)$ and $g(\gamma b)$. Then, as in (3), we formally have

$$m(a) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \frac{G(1-p)}{L(1-p)} a^{-p}\, dp. \tag{8}$$

On the basis of (6) and (7) one can show that the integral (8) converges in the strip $-2 < c < 0$ and there gives the solution of the problem, provided the sought distribution function $f(a)$ is finite at $a = 0$ and has a finite dispersion. These conditions are not physically burdensome (moreover, they can be weakened).

Using the results of (3), we successively find

$$L(p) = \frac{\cos\frac{\pi p}{2}\,\Gamma(p)}{2(2\gamma)^p} \frac{p+2}{p-2} \qquad (-4 < \operatorname{Re} p < 0); \tag{9}$$

$$\frac{1}{L(1-p)} = \frac{8\gamma}{\pi}\,\frac{\cos\frac{\pi p}{2}\,\Gamma(p)}{(2\gamma)^p}\,\frac{p+1}{p-3} \qquad (1 < \operatorname{Re} p < 5). \tag{10}$$

From these formulas, analogously to how this was done in (3), it can be proved that the solution of the integral equation (6) is determined by the relations

$$m(a) = \frac{4}{\pi}\left\{\frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{p+1}{p-3}\cos\frac{\pi p}{2}\Gamma(p)\delta(p)a^{-p}\,dp\right\}, \qquad -2 < c < 0; \tag{11}$$

$$\delta(p) = \int_0^\infty g\left(\frac{x}{2}\right) x^{-p}\,dx, \qquad 1 < \operatorname{Re} p < 5. \tag{12}$$

Here one first finds $\delta(p)$ from (12), then $\delta(p)$ is analytically continued to the strip $-2 < \operatorname{Re} p < 0$, and finally $m(a)$ is computed by (11).

4. Let us illustrate the inversion formulas (11)–(12). In view of (6) and (7), the particle spectrum

$$m_0(a) = c_0 a^2 e^{-a}, \qquad c_0 = Nr^3 \tag{13}$$

(N is the concentration, $\bar{r}$ is the mean particle radius) corresponds to the indicatrix

$$g_0\left(\frac{x}{2}\right) = c_0\vartheta_0(x), \qquad \vartheta_0(x) = \frac{x^6 + 5x^4}{(1+x^2)^3}. \tag{14}$$

Let us invert it by formulas (11)–(12). Using the properties of Euler integrals, we find

$$\delta(p) = c_0\,\frac{\pi p(p-3)}{4\cos\pi p/2}, \qquad m(a) = \frac{c_0}{2\pi i}\int_{c-i\infty}^{c+i\infty}\Gamma(p+2)a^{-p}\,dp = c_0 a^2 e^{-a} \quad (c > -2), \tag{15}$$

i.e., indeed, $m(a) = m_0(a)$.

5. We now turn to the case of a tabular specification of the indicatrix. Suppose that from experiment the quantities $g(x_i/2)$ $(0 < x_1 < \ldots < x_m < 2\gamma)$ have been obtained and that, on the basis of these data, for $x > 1$ constants C and D have been determined which describe the "tail" of the function $g(x/2)$,

$$g\left(\frac{x}{2}\right) \simeq C + \frac{D}{x^2} \qquad (x > 1). \tag{16}$$

Then

$$\delta(p) \simeq \sum_{j=1}^{m} g\left(\frac{x_j}{2}\right) x_j^{-p}\, \Delta x_j + C\,\frac{(2\gamma)^{1-p}}{p-1} + D\,\frac{(2\gamma)^{-1-p}}{p-1}, \qquad \sum_{j=1}^{m} \Delta x_j = 2\gamma. \tag{17}$$

Denote by $\widetilde{m}(a)$ the value $m(a)$ found from formula (11) for $\delta(p)$ from (17). We have

$$\widetilde{m}(a) = \frac{4}{\pi}\left\{\sum_{j=1}^{m} g\left(\frac{x_j}{2}\right) \chi(a x_j)\, \Delta x_j + 2\gamma C\, \chi_0(2\gamma a) + \frac{D}{2\gamma}\, \chi_2(2\gamma a)\right\}, \tag{18}$$

where

$$\chi(y) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{p+1}{p-3}\,\Gamma(p)\cos\frac{\pi p}{2}\, y^{-p}\, dp,$$

$$\chi_0(y) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{p+1}{(p-1)(p-3)}\,\Gamma(p)\cos\frac{\pi p}{2}\, y^{-p}\, dp, \tag{19}$$

$$\chi_2(y) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \frac{1}{p-3}\,\Gamma(p)\cos\frac{\pi p}{2}\, y^{-p}\, dp \qquad (-2 < c < 0).$$

On the basis of the appendices to (3) and (4) we compute the inverse Mellin transforms for the functions in (19). We have

$$\frac{p+1}{p-3} = 1 + \frac{4}{p-1} + \frac{8}{(p-1)(p-2)} + \frac{8}{(p-1)(p-2)(p-3)} \tag{20}$$

and, therefore,

$$\chi(y) = \left(1 - \frac{8}{y^2}\right)\cos y + \left(\frac{8}{y^3} - \frac{4}{y}\right)\sin y + \frac{1}{3}. \tag{21}$$

By analogy we find

$$\chi_0(y) = \frac{\chi(y) - \omega_0(y)}{2}, \qquad \chi_2(y) = \frac{\chi(y) - \omega_2(y)}{4}, \tag{22}$$

$$\omega_0(y) = 1 + \cos y - 2\frac{\sin y}{y}, \qquad \omega_2(y) = \cos y - 1.$$

6. Let us illustrate the inversion formulas of Sec. 5. Consider separate values of the indicatrix (14) as the result of an experiment. Obviously,

$$\vartheta_0(x) = 1 + \frac{2}{x^2} + O\left(\frac{1}{x^4}\right). \tag{23}$$

Hence, $C = c_0$ and $D = 2c_0$. Put

$$\Delta x_j = \frac{2\gamma}{m}, \qquad 2\gamma = 4, \qquad m = 10, \qquad x_j = 0.4j - 0.2 \quad (j = 1, \dots, 10). \tag{24}$$

Then the relation to be checked is

$$a^2 e^{-a} \simeq \frac{\widetilde{m}_0(a)}{c_0} = \frac{4}{\pi}\left\{0.4\sum_{j=1}^{10}\vartheta(x_j)\chi(ax_j) + 4\chi_0(4a) + \frac{1}{2}\chi_2(4a)\right\}. \tag{25}$$

Calculations show that it is satisfied with an error not exceeding 10%.

7. The indicatrix $g(x/2)$ is defined only for $0 \le x \le 4\bar{\rho}$ $(0 \le b \le 1)$,

$$x = 4\bar{\rho}\sin\frac{\beta}{2}, \qquad \bar{\rho} = \frac{\gamma}{2} = \frac{2\pi\bar{r}}{\lambda}. \tag{26}$$

The values of the function $g(\gamma b)$ for $b > 1$ are, in essence, superfluous for the problem; they have no physical meaning, and they cannot be found experimentally. But by virtue of the mathematical apparatus used (which employs the Mellin transform of $g(\gamma b)$, referring to an infinite interval), they are needed for calculating $\widetilde{m}(a)$ by (18).

The integral equation (6) determines a unique continuation of the function $g(\gamma b)$ to $b > 1$. However, this continuation can be computed only if the spectrum of the system under study is known. Thus, for a gamma distribution of particles,

$$f_\mu(a) = c_0\frac{(\mu+1)^{\mu+1}}{\Gamma(\mu+1)}a^\mu e^{-(\mu+1)a}, \tag{27}$$

according to (6), we obtain

$$g_\mu\left(\frac{x}{2}\right) = \frac{c_0}{2}\frac{\mu+2}{\mu+1} + \frac{2c_0}{x^2} + O\left(\frac{1}{x^{2[\mu/2]+4}}\right) \quad (x \text{ arbitrary}). \tag{28}$$

For $0 \leq x \leq 4\bar{\rho}$ this function is the indicatrix of the system under consideration. The extrapolation that we used of the indicatrix $g(x/2)$ to $x > 4\bar{\rho}$ by means of formula (16) is justified by the fact that, for a broad set of spectra (27), the true continuation of the indicatrix imposed by equation (6) differs little from a function of the form (16), if x is sufficiently large. Hence, the arbitrariness associated with the choice of the extrapolating function cannot serve as a source of large errors. Thus, the computation of $\widetilde{m}(a)$ from (18) can be carried out in the case of sufficiently large $\bar{\rho}$. Physically this is explained by the fact that only for such $\bar{\rho}$ does the indicatrix differ from the Rayleigh one, and only then is inversion possible.

Let us estimate the quantity $\bar{\rho}$. From (16) and (26) it follows that

$$\bar{\rho} > \frac{1}{4} \qquad \left(\gamma > \frac{1}{2}\right). \tag{29}$$

The estimate (29) is, generally speaking, too low. In fact, the main requirement for the validity of the representation (16) consists in the absence of sharp extrema of $g(x/2)$ for $x > 4\bar{\rho}$. In particular, the indicatrix $g_0(x/2)$ from (14) has a single positive extremum—the maximum $x_m = \sqrt{5}$, i.e., in the present case one must take $\bar{\rho} > \sqrt{5}/4$. In practice, when there is a single maximum x_m of the indicatrix $g(x/2)$, it is recommended to take

$$\bar{\rho} \simeq (0.4 - 0.5)x_m \qquad (\gamma \simeq (0.8 - 1)x_m). \tag{30}$$

We note that in (24) $\gamma = 2$ was adopted for $x_m = \sqrt{5}$. The exact inversion of equation (6) made it possible to eliminate a source of large errors that arise in solving Fredholm integral equations of the first kind. The formula for the particle spectrum (18), in the case of a tabulated indicatrix, contains only those approximate equalities which inevitably arise when using information on scattered light obtained experimentally. Computation by formula (18) is noticeably simplified if one uses tables of the functions $\varkappa(y)$, $\varkappa_0(y)$, and $\varkappa_2(y)$, compiled by us.

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