Methods of integral geometry and finding the relative orientation of identical particles arbitrarily arranged in a plane from their projections onto a straight line

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1. Introduction and exact formulation of the problem. Electron-microscopic studies of the structure of asymmetric biological particles have raised the question (see Refs. 1, 2, and 6) of how to find the spatial orientation of arbitrarily arranged particles of unknown structure from their projections.

Suppose that $\rho(y_1, y_2, y_3)$ is the electron density distribution function of the particle and $\rho_\omega(y_1, y_2, y_3)$ is the electron density distribution function for a particle, which is obtained as a result of a rotation ω of the initial particle. The task is to find the transformations $\omega_2, \ldots, \omega_n$ if we know the projection

$$p_{\omega_i}(y_1, y_2) = \int \rho_{\omega_i}(y_1, y_2, y_3)dy_3, \quad i = 1, 2, \ldots, n, \quad \omega_1 = id.$$

By π we denote the plane $y_3 = 0$. The method of Refs. 1, 2, and 6 allows the transformation ω_i to be reconstructed when the intersection of the planes $\pi, \omega_2^{-1}\pi, \ldots, \omega_n^{-1}\pi$ is not a straight line. This condition is not always satisfied, however, in a real situation, in particular in electron-microscopic studies of biological particles. Suppose, for example, that the particle under study extends in one direction and that if such particles are placed on a substrate, the direction in which they extend is parallel to the plane of the film.

Since the direction in which the particle extends is clearly visible on the projection, we can assume that the particle rotates through unknown angles $\varphi_1, \ldots, \varphi_n$ around a preferred axis and is projected onto a plane.

The center of gravity of the particle is projected to the center of gravity of the projection. We consider a planar section that passes through the center of gravity of the particle and is perpendicular to the axis around which the particle rotates (see Fig. 1). Suppose that x_1 and x_2 are the coordinates in the plane of the cross section, where the center of gravity of the plane section of the particle is situated at the point (0, 0). By $\rho(x_1, x_2)$ we denote the distribution function of the plane section of the particle.

We consider the following problem: a plane particle rotates through unknown angles $\varphi_1, \ldots, \varphi_n$ around its center of gravity and is projected onto the straight line $x_2 = 0$. Find the relative angles $\varphi_k - \varphi_1$, $k = 2, \ldots, n$. Clearly, we can assume that $\varphi_1 = 0$.

In this paper we propose a method that allows the angles $\varphi_2, \ldots, \varphi_n$ to be reconstructed unambiguously for an asymmetric particle for $n \geq 7$.

Once the angles $\varphi_2, \ldots, \varphi_n$ have been found, we can carry out a three-dimensional reconstruction of the initial structure from projections in already known directions (see Ref. 3).

2. Properties of the moments of projections. The distribution function $\rho_\varphi(x_1, x_2)$ of a particle rotated through an angle φ counterclockwise is given by

$$\rho_\varphi(x_1, x_2) = \rho(x_1 \cos\varphi + x_2 \sin\varphi, \ -x_1 \sin\varphi + x_2 \cos\varphi).$$

For the projection $p_\varphi(x_1) = \int \rho_\varphi(x_1, x_2)dx_2$ of the function $\rho_\varphi(x_1, x_2)$ on to the straight line $x_2 = 0$ we determine the k-th moment $M_k(\varphi)$ from the equation

$$M_k(\varphi) = \int p_\varphi(x_1)x_1^k dx_1. \tag{1}$$

The entire analysis is based on the fact that $M_k(\varphi)$ is a uniform trigonometric polynomial of degree k, i.e.,

$$M_k(\varphi) = \lambda_{k0}\cos^k\varphi + \lambda_{k-1,1}\cos^{k-1}\varphi\sin\varphi + \ldots + \lambda_{0k}\sin^k\varphi.$$

Upon changing variables $y_1 = x_1\cos\varphi + x_2\sin\varphi$, $y_2 = -x_1\sin\varphi + x_2\cos\varphi$ (and, therefore, $x_1 = y_1\cos\varphi - y_2\sin\varphi$) in Eq. (1), we obtain

$$\begin{aligned} M_k(\varphi) &= \int \rho(y_1, y_2)(y_1\cos\varphi - y_2\sin\varphi)^k dy_1 dy_2 \\ &= \left(\int \rho(y_1, y_2)y_1^k dy_1 dy_2\right)\cos^k\varphi + \left(-C_k^1 \int \rho(y_1, y_2)y_1^{k-1}y_2 dy_1 dy_2\right)\cos^{k-1}\varphi\sin\varphi \\ &+ \ldots + \left((-1)^k \int \rho(y_1, y_2)y_2^k dy_1 dy_2\right)\sin^k\varphi. \end{aligned} \tag{1'}$$

These equations for the moments of projections were first obtained by Gel'fand and Graev in 1961 (Paley–Wiener theorem for the Radon transformation, see Refs. 4 and 5); Gel'fand proposed that they be called the Cavalieri conditions, because at $k = 0$ the condition $M_0(\varphi) = \text{const}$ expresses the familiar Cavalieri principle: the area of a body can be calculated from the length of its cross sections by any bundle of parallel straight lines.

It should be pointed out that hitherto only the Radon transformation (in a plane and in space) and the Radon rotation formula have been used in problems of three-

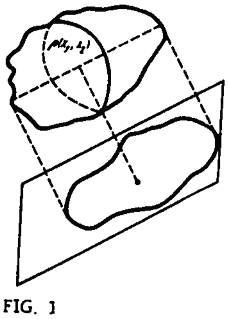

FIG. 1

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dimensional reconstruction. Undoubtedly, not only the Paley-Wiener theorem but also other results and methods of integral geometry (see Refs. 4 and 5) will prove useful in applied problems.

A uniform trigonometric polynomial of degree k is determined uniquely by the values that it assumes for any k+1 values of the argument $\varphi_1, \ldots, \varphi_{k+1}$ $(0 \leq \varphi_i < 2\pi)$ such that $\varphi_i - \varphi_j \neq \pm\pi$. [This last condition is necessary, since $M_k(\varphi \pm \pi) = (-1)^k M_k(\varphi)$.] Indeed, we know the values of the function

$$\frac{M_k(\varphi)}{\cos^k\varphi} = \lambda_{0k} \tan^k \varphi + \lambda_{1,k-1} \operatorname{tg}^{k-1}\varphi + \ldots + \lambda_{k0}$$

for k+1 values of the argument $\varphi_1, \ldots, \varphi_{k+1}$, under the condition $\tan \varphi_i \neq \tan \varphi_j$, and as is known a polynomial of degree no higher than k is determined uniquely by its value at k+1 different points.

Considering several moments simultaneously, we obtain a system of equations for their coefficients and angles φ_i. As n increases, this system becomes highly overdetermined but it does allow all the angles φ_i to be found.

3. Finding the angles $\varphi_2, \ldots, \varphi_n$ for $n \geq 7$ for an asymmetric particle. Since the center of gravity of the projection $p_\varphi(x_1)$ lies at the point $x_1 = 0$, we have $M_1(\varphi) = \int p_\varphi(x_1)x_1dx_1 = 0$. For an asymmetric particle higher moments are generally not identically equal to zero. Henceforth, to avoid confusion we denote $m_k(i)$ to be a number equal to $\int p_{\varphi_i}(x_1)x_1^k dx_1 \equiv M_k(\varphi)$.

We consider the system of equations

$$\begin{aligned} &\lambda_{20}\cos^2\varphi_i + \lambda_{11}\cos\varphi_i \sin\varphi_i + \lambda_{02}\sin^2\varphi_i = m_2(i), \\ &\lambda_{30}\cos^3\varphi_i + \lambda_{21}\cos^2\varphi_i \sin\varphi_i + \lambda_{12}\cos\varphi_i \sin^2\varphi_i + \lambda_{03}\sin^3\varphi_i = m_3(i). \end{aligned} \tag{2}$$

Since $\varphi_1 = 0$, the symbols $\lambda_{20} = m_2(1)$ and $\lambda_{30} = m_3(1)$ are known numbers. We have obtained a system of $2(n-1)$ equations for $5 + (n-1) = n+4$ unknowns $\lambda_{11}, \lambda_{02}; \lambda_{21}, \lambda_{12}, \lambda_{03}; \varphi_2, \ldots, \varphi_n$. For $n \geq 7$, therefore, we have an overdetermined system of equations, which we solve to find the angles $\varphi_2, \ldots, \varphi_n$.

Realistically, we can look for the minima of the nonnegative function

$$\sum_{i=2}^{n} (\lambda_{20}\cos^2\varphi_i + \lambda_{11}\cos\varphi_i \sin\varphi_i + \lambda_{02}\sin^2\varphi_i - m_2(i))^2$$

$$+ \sum_{i=2}^{n} (\lambda_{30}\cos^3\varphi_i + \lambda_{21}\cos^2\varphi_i \sin\varphi_i + \lambda_{12}\cos\varphi_i \sin^2\varphi_i + \lambda_{03}\sin^3\varphi_i - m_3(i))^2.$$

It is sufficient to assume n=7. This will then be a function of 11 variables.

4. Final remarks.

a. This method can be simplified considerably if w also know the values of several angles. Thus, upon fur ing the electron microscope with a goniometer, we can rotate the film several times with the object and take a photograph. For example, suppose that the angles φ_2, and φ_4 are known in addition to the other quantities. So ing the system of linear equations (2), where i=1, 2, 3, 4 $(\varphi_1 = 0)$, we then find $M_2(\varphi)$ and $M_3(\varphi)$. We solve the equat $M_2(\varphi) = m_2(i)$ in order to determine the other angles φ_i (i ≥ In general, this equation has four solutions: $\psi_i^{(1)}, \psi_i^{(2)}, \psi_i^{(1)}$ $\psi^{(2)} + \pi$. The solution that satisfies the equation $M_3(\varphi) = m_3(i)$ is the value of the angle φ_i which we are seeking.

b. Using higher moments, we can in similar fashi find the relative position of identical plane particles wl have a finite symmetry group.

c. Suppose that

$$\check{f}(\omega, p) = \int\int f(x_1, x_2)\delta(x_1\omega_1 + x_2\omega_2 - p)dx_1dx_2, \quad |\omega| = 1,$$

is the Radon transformation of a finite function f(x). It can then be shown that in order to find f(x) to within rot tion or reflection relative to a straight line, we need no necessarily know how $\check{f}(\omega, p)$ depends on ω. It is suffici to know the set of functions $\varphi_\alpha(p)$ of one variable, whicl depends on the parameter α, so that for each value of α there is a value $\omega(\alpha)$ for which $\varphi_\alpha(p) = \check{f}[\omega(\alpha), p]$, but th law of the correspondence $\alpha \to \omega(\alpha)$ is not known.

A more exact formulation is as follows. We consid $\check{f}(\omega, p)$ as a function of ω: $\check{F}_f(\omega)$ with values in the spac of functions of the variable p. To reconstruct f(x), it would then be sufficient to know only the set of values o $\check{F}_f(\omega)$ and not the function itself. This is done in two sta 1) all the moments $M_k(\varphi)$ are found; 2) Eq. (1') means t the moments $M_k(\varphi)$ determine the moments of the funct $f(x_1, x_2)$. We know that a finite function is determined uniquely by its moments.

The function f(x) can thus be reconstructed immedi from the moments, without finding the angles.

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