International Tables for Crystallography (2006). Vol. C, Figure 2.6.1.4, p. 94.

gyration R_g [slope of the main maximum of $I(h)$ or the second moment of $p(r)$] constant.

The scattering function of a sphere with $R = 65$ is shown in Fig. 2.6.1.2 [dashed line, $\log I(0)$ normalized to 12]. We see distinct minima which are typical for particles of high symmetry. We can determine the size of the sphere directly from the position of the zeros h_{01} and h_{02} (Glatter, 1972).

$$R \simeq \frac{4.493}{h_{01}} \quad \text{or} \quad R \simeq \frac{7.725}{h_{02}} \qquad (2.6.1.39)$$

or from the position of the first side maximum ($R_g \simeq 4.5/h_1$). The minima are considerably flattened in the case of cubes (full line in Fig. 2.6.1.2). The corresponding differences in real space are not so clear-cut (Fig. 2.6.1.3). The $p(r)$ function of the sphere has a maximum near $r = R = D/2$ ($x \simeq 0.525$) and drops to zero like every PDDF at $r = D$, where D is the maximum dimension of the particle – here the diameter. The $p(r)$ for the cube with the same R_g is zero at $r \simeq 175$. The function is very flat in this region. This fact demonstrates the problems of accuracy in this determination of D when we take into account experimental errors. In any case, this accuracy will be different for different shapes.

Any deviation from spherical symmetry will shift the maximum to smaller r values and the value for D will increase [$I(0)$ and R_g constant!]. A comparison of PDDF's for a sphere, an oblate ellipsoid of revolution (axial ratio 1:1:0.2), and a prolate ellipsoid of revolution (1:1:3) is shown in Fig. 2.6.1.4. The more we change from the compact, spherical structure to a two- and one-dimensionally elongated structure, the more the maximum shifts to smaller r values and at the same time we have an increase in D. We see that $p(r)$ is a very informative function. The interpretation of scattering functions in reciprocal space is hampered by the highly abstract nature of this domain. We can see this problem in Fig. 2.6.1.5, where the scattering functions of the sphere and the ellipsoids in Fig. 2.6.1.4 are plotted. A systematic discussion of the features of $p(r)$ can be found elsewhere (Glatter, 1979, 1982*b*).

Rod-like particles. The first example of a particle elongated in one direction (prolate ellipsoid) was given in Figs. 2.6.1.4 and 2.6.1.5. An important class is particles elongated in one

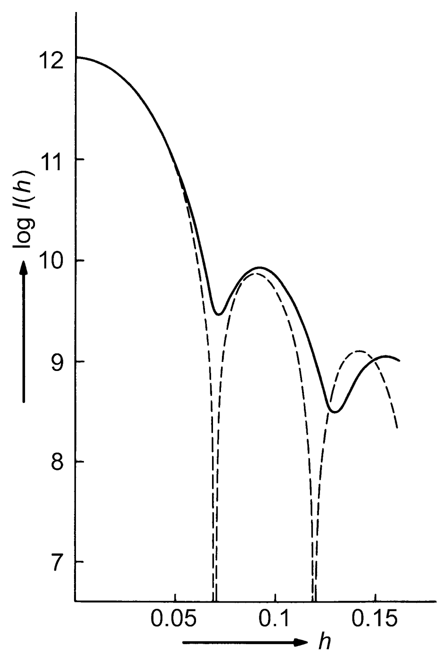

Fig. 2.6.1.2. Comparison of the scattering functions of a sphere (- - - -) and a cube (———) with same radius of gyration.

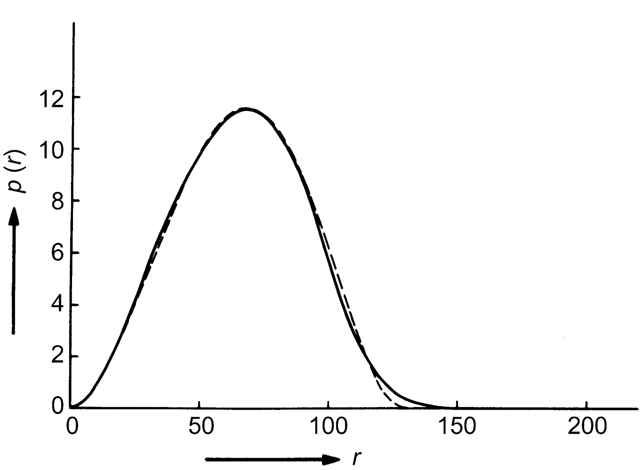

Fig. 2.6.1.3. Distance distribution function of a sphere (- - - -) and a cube (———) with the same radius of gyration and the same scattering intensity at zero angle.

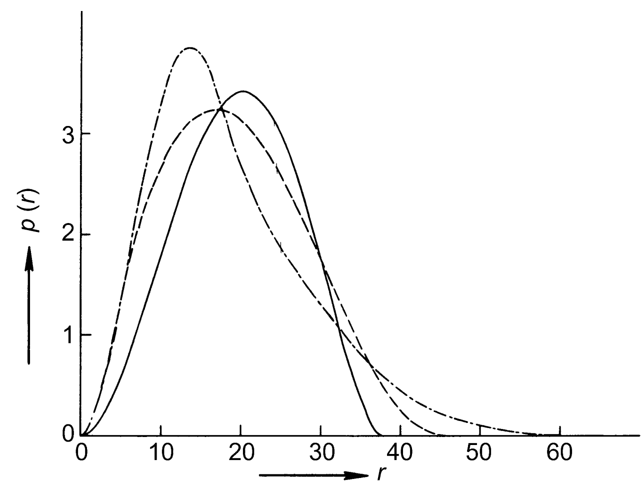

Fig. 2.6.1.4. Comparison of the $p(r)$ function of a sphere (———), a prolate ellipsoid of revolution 1:1:3 (—·—·—), and an oblate ellipsoid of revolution 1:1:0.2 (- - - -) with the same radius of gyration.

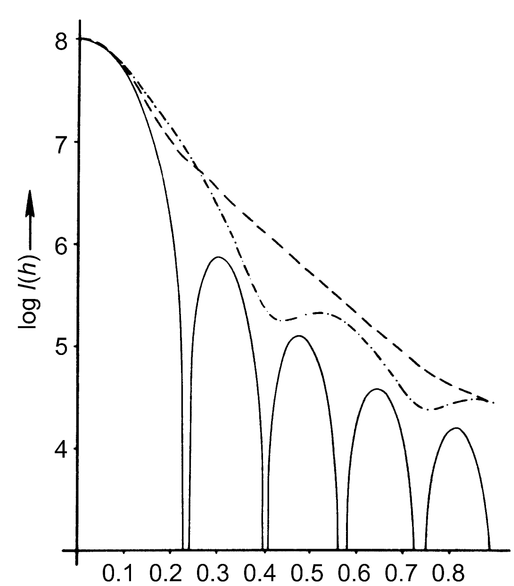

Fig. 2.6.1.5. Comparison of the $I(h)$ functions of a sphere, a prolate, and an oblate ellipsoid (see legend to Fig. 2.6.1.4).