

2.6. SMALL-ANGLE TECHNIQUES

Fournet, 1955; Glatter, 1979). The inverse transform to (2.6.1.9) is given by

$$p(r) = \frac{1}{2\pi^2} \int_0^\infty I(h)hr \sin(hr) dh \quad (2.6.1.10)$$

or by

$$V\gamma(r) = \frac{1}{2\pi^2} \int_0^\infty I(h)h^2 \frac{\sin hr}{hr} dh. \quad (2.6.1.11)$$

The function $p(r)$ is directly connected with the measurable scattering intensity and is very important for the solution of the inverse scattering problem. Before working out details, we should first discuss equations (2.6.1.9) and (2.6.1.10).

The PDDF can be defined as follows: the function $p(r)$ gives the number of difference electron pairs with a mutual distance between r and $r + dr$ within the particle. For homogeneous particles (constant electron density), this function has a simple and clear geometrical definition.

Let us subdivide the particle into a very large number of identical small volume elements. The function $p(r)$ is proportional to the number of lines with a length between r and $r + dr$ which are found in the combination of any volume element i with any other volume element k of the particle (see Fig. 2.6.1.1). For $r = 0$, there is no other volume element, so $p(r)$ must be zero, increasing with r^2 as the number of possible neighbouring volume elements is proportional to the surface of a sphere with radius r . Starting from an arbitrary point in the particle, there is a certain probability that the surface will be reached within the distance r . This will cause the $p(r)$ function to drop below the r^2 parabola and finally the PDDF will be zero for all $r > D$, where D is the maximum dimension of the particle. So $p(r)$ is a distance histogram of the particle. There is no information about the orientation of these lines in $p(r)$, because of the spatial averaging.

In the case of inhomogeneous particles, we have to weight each line by the product of the difference in electron density $\Delta\rho$, and the differential volume element, dV . This can lead to negative contributions to the PDDF.

We can see from equation (2.6.1.9) that every distance r gives a $\sin(hr)/(hr)$ contribution with the weight $p(r)$ to the total scattering intensity. $I(h)$ and $p(r)$ contain the same information, but in most cases it is easier to analyse in terms of distances than in terms of $\sin(x)/x$ contributions. The PDDF could be computed exactly with equation (2.6.1.10) if $I(h)$ were known for the whole reciprocal space.

For $h = 0$, we obtain from equation (2.6.1.9)

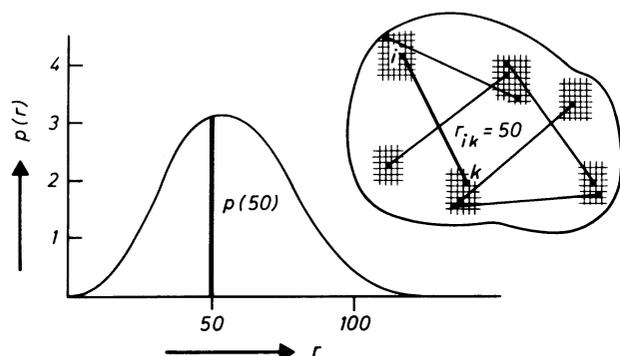


Fig. 2.6.1.1. The height of the $p(r)$ function for a certain value of r is proportional to the number of lines with a length between r and $r + dr$ within the particle.

$$I(0) = I(\overline{\Delta\rho})^2 V^2 = 4\pi \int_0^\infty p(r) dr, \quad (2.6.1.12)$$

i.e. the scattering intensity at h equal to zero is proportional to the area under the PDDF. From equation (2.6.1.11), we find

$$V\gamma(0) = \frac{1}{2\pi^2} \int I(h)h^2 dh = V\overline{\Delta\rho^2} \quad (2.6.1.13)$$

(Porod, 1982), *i.e.* the integral of the intensity times h^2 is related to the mean-square fluctuation of the electron density irrespective of the structure. We may modify the shape of a particle, the scattering function $I(h)$ might be altered considerably, but the integral (2.6.1.13) must remain invariant (Porod, 1951).

$$\text{Invariant } Q = \int_0^\infty I(h)h^2 dh. \quad (2.6.1.14)$$

2.6.1.3. Monodisperse systems

In this subsection, we discuss scattering from monodisperse systems, *i.e.* all particles in the scattering volume have the same size, shape, and internal structure. These conditions are usually met by biological macromolecules in solution. Furthermore, we assume that these solutions are at infinite dilution, which is taken into account by measuring a series of scattering functions at different concentrations and by extrapolating these data to zero concentration. We continue with the notations defined in the previous subsection, which coincide to a large extent with the notations in the original papers and in the textbooks (Guinier & Fournet, 1955; Glatter & Kratky, 1982). There is a notation created by Luzzati (1960) that is quite different in many details. A comparison of the two notations is given in the Appendix of Pilz, Glatter & Kratky (1980).

The particles can be roughly described by some parameters that can be extracted from the scattering function. More information about the shape and structure of the particles can be found by detailed discussion of the scattering functions. At first, this discussion will be about homogeneous particles and will be followed by some aspects for inhomogeneous systems. Finally, we have to discuss the influence of finite concentrations on our results.

2.6.1.3.1. Parameters of a particle

Total scattering length. The scattering intensity at $h = 0$ must be equal to the square of the number of excess electrons, as follows from equations (2.6.1.7) and (2.6.1.12):

$$I(0) = (\Delta\rho)^2 V^2 = 4\pi \int_0^\infty p(r) dr. \quad (2.6.1.15)$$

This value is important for the determination of the molecular weight if we perform our experiments on an absolute scale (see below).

Radius of gyration. The electronic radius of gyration of the whole particle is defined in analogy to the radius of gyration in mechanics:

$$R_g^2 = \frac{\int \rho(r_i)r_i^2 dV_i}{\int \rho(r_i) dV_i}. \quad (2.6.1.16)$$

It can be obtained from the PDDF by