solution. This problem is far from being trivial, but it can be solved with standard routines (Glatter, 1977*a*,*b*; Tikhonov & Arsenin, 1977).

The whole process of data evaluation is shown in Fig. 2.6.1.14. Similar routines cannot be used in crystallography (periodic structures) because there exists no estimate for $D_{\max}$ [equation (2.6.1.57)].

Maximum particle dimension. The sampling theorem of Fourier transformation (Shannon & Weaver, 1949; Bracewell, 1986) gives a clear answer to the question of how the size of the particle D is related to the smallest scattering angle h_1. If the scattering curve is observed at increments $\Delta h \leq h_1$ starting from a scattering angle h_1, the scattering data contain, at least theoretically, the full information for all particles with maximum dimension D

$$D \leq \pi/h_1. \tag{2.6.1.62}$$

The first application of this theorem to the problem of data evaluation was given by Damaschun & Pürschel (1971*a*,*b*). In practice, one should always try to stay below this limit, *i.e.*

$$h_1 < \pi/D \quad \text{and} \quad \Delta h \ll h_1, \tag{2.6.1.63}$$

taking into account the loss of information due to counting statistics and smearing effects. An optimum value for $\Delta h = \pi/(6D)$ is claimed by Walter, Kranold & Becherer (1974).

Information content. The number of *independent* parameters contained in a small-angle scattering curve is given by

$$N_{\max} \leq h_2/h_1, \tag{2.6.1.64}$$

with h_1 and h_2 being the lower and upper limits of h. In practice, this limit certainly depends on the statistical accuracy of the data. It should be noted that the number of functions N in equations (2.6.1.58) to (2.6.1.60) may be larger than $N_{\max}$ because they are not independent. They are correlated by the stabilization routine. An example of this problem can be found in Glatter (1980*a*).

Resolution. There is no clear answer to the question concerning the smallest structural details, *i.e.* details in the $p(r)$ function that can be recognized from an experimental scattering function. The limiting factors are the maximum scattering angle h_2, the statistical error $\sigma(h)$, and the weighting functions $P(t)$, $Q(x)$, and $W(\lambda')$ (Glatter, 1982*a*). The resolution of standard experiments is not better than approximately 10% of the maximum dimension of the particle for a monodisperse system. In the case of polydisperse systems, resolution can be defined as the minimum relative peak distance that can be resolved in a bimodal distribution. We know from simulations that this value is of the order of 25%.

Special transforms. The PDDF $p(r)$ or the size distribution function $D(R)$ is related to $I(h)$ by equations (2.6.1.9) or (2.6.1.54), (2.6.1.55). In the special case of particles elongated in one direction (like cylinders), we can combine equations (2.6.1.41) and (2.6.1.43) and obtain

$$I(h) = 2\pi^2 L \int_0^\infty p_c(r) \frac{J_0(hr)}{h}\, \mathrm{d}r. \tag{2.6.1.65}$$

This Hankel transform can be used in the indirect transformation method for the calculation of $\psi_\nu(h)$ in (2.6.1.59). Doing this, we immediately obtain the PDDF of the cross section $p_c(r)$ from the smeared experimental data. It is not necessary to know the length L of the particle if the results are not needed on an absolute scale. For this application, we only need the information that the scatterers are elongated in one direction with a constant cross section. This information can be found from the overall PDDF of the particle or can be *a priori* information from other experiments, like electron microscopy. The estimate for the maximum dimension $D_{\max}$ (2.6.1.57) is related to the cross

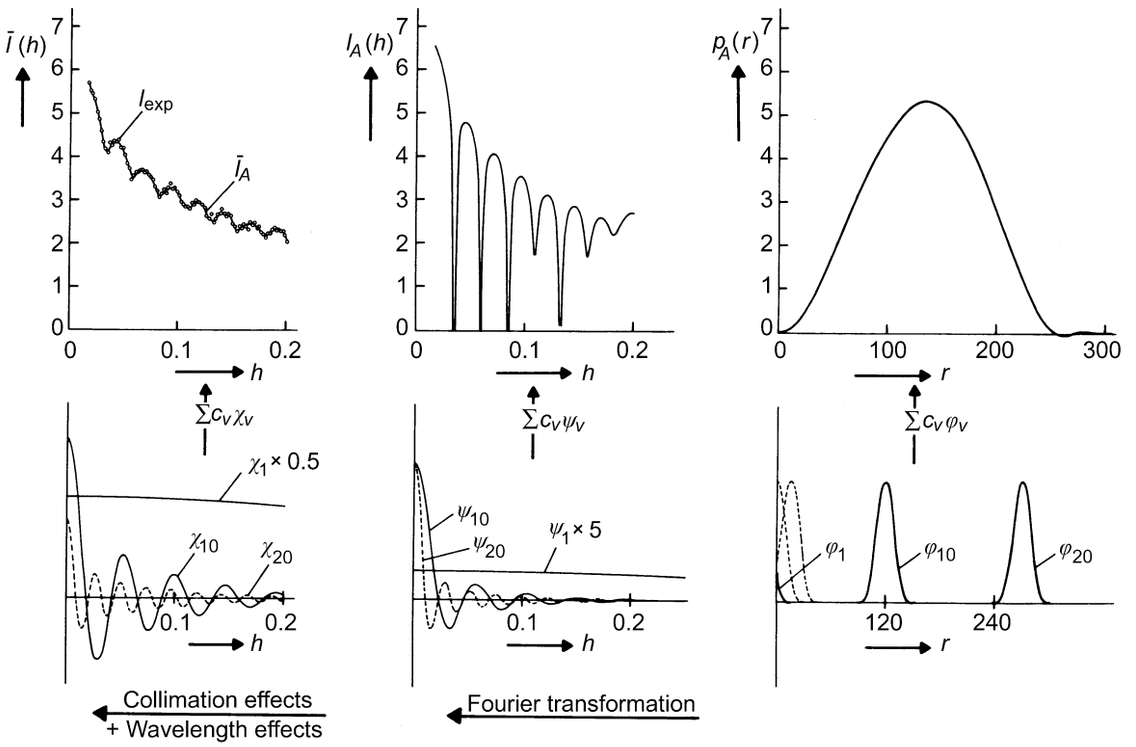

Fig. 2.6.1.14. Function systems $\varphi_\nu(r)$, $\Psi_\nu(h)$, and $\chi_\nu(h)$ used for the approximation of the scattering data in the indirect transformation method.

references