space, possibly looped, and ending on the point with coordinates (h, k).

This solution can also be obtained by iteration of the Green-function integral equation, the integrals being evaluated by means of suitably chosen contours on the complex k_z plane (Fujiwara, 1959), as well as by expansion of the scattering matrix (Fujimoto, 1959).

Clearly, two or more of the ζ_i will, in general, be equal in nearly all of the terms in equation (5.2.13.1*a*). Confluence is, however, readily described, the divided differences of arbitrary order transforming into differentials of the same order (Moodie, 1972).

The physical picture that emerges from equation (5.2.13.1*a*) is that of n-fold scattering, the initial wave being turned through $n-1$ intermediate states, processes that can be presented by scattering diagrams in reciprocal space (Gjønnes & Moodie, 1965).

For a given scattering vector, constituent functions are evaluated for all possible paths in three dimensions, and those functions are then summed over l. There are therefore two distinct processes by which upper-layer lines can perturb wavefunctions in the zone, namely: by scattering out of the zone and then back in; and by intrusion of the effective shape function from another zone, the latter process being already operative in the first Born, or kinematical approximation.

The constituent functions to be evaluated can be transformed into many forms. One of the more readily described is that which assigns to each diagram an effective dynamical shape function. If there are no loops in the diagram of order n, this effective shape function is the $(n+1)$th divided difference of the constituent phase-shifted kinematical shape transforms. For general diagrams, divided differences in loops are replaced by the corresponding differentials. The resulting function is multiplied by the convolution of the contributing structure amplitudes and diagrams of all orders summed (Moodie, 1972).

While scattering diagrams have no utility in numerical work, they find application in the analysis of symmetries, for instance in the determination of the presence or absence of a centre of inversion [for a recent treatment, see Moodie & Whitfield (1995)] and in the detection of screw axes and glide planes (Gjønnes & Moodie, 1965). Methods for the direct determination of all space groups are described by Goodman (1975) and by Tanaka *et al*. (1983) (see Section 2.5.3).

Equation (5.2.13.1*a*) can be rewritten in a form particularly suited to the classification of approximations, and to describing the underlying symmetry of the formulation. The equation is written for compactness as

$$U_n(h) = E_n(h) Z_n(\zeta),$$

so that $E_n(h)$ depends only on crystal structure and $Z_n(\zeta)$ only on diffraction geometry. A transformation (Cowley & Moodie, 1962) involving bialternants leads to

$$U_n = \sum_{r=0}^{\infty} E_n(h)\left[(2\pi i T)^{n+r}/(n+r)!\right] h_r(\zeta, \zeta_1 \ldots \zeta_{n-1}), \qquad (5.2.13.1b)$$

where h_r is the complete homogeneous symmetric polynomial function of n variables of order r.

Upper-layer-line effects can, of course, be calculated in any of the formulations.

5.2.14. Approximations

So far, only the familiar first Born and two-beam approximations and the projection approximation have been mentioned. Several others, however, have a considerable utility.

A high-voltage limit can be calculated in standard fashion to give

$$U_{HVL}(h,k) = \mathscr{F} \exp\left\{-i\sigma_c \int_0^T \varphi(x,y,z)\, \mathrm{d}z\right\}, \qquad (5.2.14.1)$$

where $\mathscr{F}$ is the Fourier transform operator, and $\sigma_c = 2\pi m_0 e \lambda_c / h^2$ with $\lambda_c = (h/m_0 c)$, the Compton wavelength. The phase-grating approximation, which finds application in electron microscopy, involves the assumption that equation (5.2.14.1) has some range of validity when σ_c is replaced by σ. This is equivalent to ignoring the curvature of the Ewald sphere and can therefore apply to thin crystals [see Section 2.5.2 and *IT* C (1999, Section 4.3.8)].

Approximations that involve curtailing the number of beams evidently have a range of validity that depends on the size of the unit cell. The most explored case is that of three-beam interactions. Kambe (1957) has demonstrated that phase information can be obtained from the diffraction data; Gjønnes & Høier (1971) analysed the confluent case, and Hurley & Moodie (1980) have given an explicit inversion for the centrosymmetric case. Analyses of the symmetry of the defining differential equation, and of the geometry of the noncentrosymmetric case, have been given by Moodie *et al*. (1996, 1998).

Niehrs and his co-workers (*e.g*. Blume, 1966) have shown that, at or near zones, effective two-beam conditions can sometimes obtain, in that, for instance, the central beam and six equidistant beams of equal structure amplitude can exhibit two-beam behaviour when the excitation errors are equal. Group-theoretical treatments have been given by Fukuhara (1966) and by Kogiso & Takahashi (1977). Explicit reductions for all admissible noncentrosymmetric space groups have been obtained by Moodie & Whitfield (1994). Extensions of such results have application in the interpretation of lattice images and convergent-beam patterns.

The approximations near the classical limit have been extensively explored [for instance, see Berry (1971)] but channelling has effectively become a separate subject and cannot be discussed here.

references