In terms of the 'Hamiltonian' of the two-dimensional system,

$$-\mathbf{H}(z) \equiv \frac{1}{2k_z}(\nabla^2_{x,\,y} + K_0^2) + \sigma\varphi,$$

the evolution operator $\mathbf{U}(z, z_0)$, defined by $\psi(z) = \mathbf{U}(z, z_0)\psi_0$, satisfies

$$i\frac{\partial}{\partial z}\mathbf{U}(z, z_0) = \mathbf{H}(z)\mathbf{U}(z, z_0), \qquad (5.2.4.1a)$$

or

$$\mathbf{U}(z, z_0) = 1 - i\int_{z_0}^{z} \mathbf{U}(z, z_1)\mathbf{H}(z_1)\,\mathrm{d}z_1. \qquad (5.2.4.1b)$$

5.2.5. Projection approximation – real-space solution

Many of the features of the more general solutions are retained in the practically important projection approximation in which $\varphi(x, y, z)$ is replaced by its projected mean value $\varphi_p(x, y)$, so that the corresponding Hamiltonian $\mathbf{H}_p$ does not depend on z. Equation (5.2.4.1*b*) can then be solved directly by iteration to give

$$\mathbf{U}_p(z, z_0) = \exp\{-i\mathbf{H}_p(z - z_0)\}, \qquad (5.2.5.1)$$

and the solution may be verified by substitution into equation (5.2.4.1*a*).

Many of the results of dynamical theory can be obtained by expansion of equation (5.2.5.1) as

$$\mathbf{U}_p \equiv \mathbf{1} - i\mathbf{H}_p(z - z_0) + \frac{i^2}{2!}\mathbf{H}_p^2(z - z_0) - \ldots,$$

followed by the direct evaluation of the differentials. Such expressions can be used, for instance, to explore symmetries in image space.

5.2.6. Semi-reciprocal space

In the derivation of electron-diffraction equations, it is more usual to work in semi-reciprocal space (Tournarie, 1962). This can be achieved by transforming equation (5.2.2.1) with respect to x and y but not with respect to z, to obtain Tournarie's equation

$$\frac{\mathrm{d}^2|U\rangle}{\mathrm{d}z^2} = -\mathbf{M}_b(z)|U\rangle. \qquad (5.2.6.1a)$$

Here $|U\rangle$ is the column vector of scattering amplitudes and $\mathbf{M}_b(z)$ is a matrix, appropriate to LEED, with $\mathbf{k}$ vectors as diagonal elements and Fourier coefficients of the potential as nondiagonal elements.

This equation is factorized in a manner parallel to that used on the real-space equation [equation (5.2.3.1)] (Lynch & Moodie, 1972) to obtain Tournarie's forward-scattering equation

$$\frac{\mathrm{d}|U^{\pm}\rangle}{\mathrm{d}z} = \pm i\mathbf{M}^{\pm}(z)|U^{\pm}\rangle, \qquad (5.2.6.1b)$$

where

$$\mathbf{M}^{\pm}(z) = \pm[\mathbf{K} + (1/2)\mathbf{K}^{-1}V(z)],$$
$$[K_{ij}] = \delta_{ij}K_i,$$

and

$$[V_{ij}] = 2k_z\sum_l V_{i-j}\exp\{-2\pi i l z\},$$

where $V_i \equiv \sigma v_i$ are the scattering coefficients and v_i are the structure amplitudes in volts. In order to simplify the electron-diffraction expression, the third crystallographic index 'l' is taken to represent the periodicity along the z direction.

The double solution involving $\mathbf{M}$ of equation (5.2.6.1*b*) is of interest in displaying the symmetry of reciprocity, and may be compared with the double solution obtained for the real-space equation [equation (5.2.3.2)]. Normally the $\mathbf{M}^+$ solution will be followed through to give the fast-electron forward-scattering equations appropriate in HEED. $\mathbf{M}^-$, however, represents the equivalent set of equations corresponding to the z reversed reciprocity configuration. Reciprocity solutions will yield diffraction symmetries in the forward direction when coupled with crystal-inverting symmetries (Section 2.5.3).

Once again we set out to solve the forward-scattering equation (5.2.6.1*a*,*b*) now in semi-reciprocal space, and define an operator $\mathbf{Q}(z)$ [compare with equation (5.2.4.1*a*)] such that

$$|U_z\rangle = \mathbf{Q}_z|U_0\rangle \quad \text{with} \quad U_0 = |0\rangle;$$

i.e., $\mathbf{Q}_z$ is an operator that, when acting on the incident wavevector, generates the wavefunction in semi-reciprocal space.

Again, the differential equation can be transformed into an integral equation, and once again this can be iterated. In the projection approximation, with $\mathbf{M}$ independent of z, the solution can be written as

$$\mathbf{Q}_p = \exp\{i\mathbf{M}_p(z - z_0)\}.$$

A typical off-diagonal element is given by $V_{i-j}/\cos\theta_i$, where θ_i is the angle through which the beam is scattered. It is usual in the literature to find that $\cos\theta_i$ has been approximated as unity, since even the most accurate measurements are, so far, in error by much more than this amount.

This expression for $\mathbf{Q}_p$ is Sturkey's (1957) solution, a most useful relation, written explicitly as

$$|U\rangle = \exp\{i\mathbf{M}_pT\}|0\rangle \qquad (5.2.6.2)$$

with T the thickness of the crystal, and $|0\rangle$, the incident state, a column vector with the first entry unity and the rest zero.

$$\mathbf{S} = \exp\{i\mathbf{M}_pT\}$$

is a unitary matrix, so that in this formulation scattering is described as rotation in Hilbert space.

5.2.7. Two-beam approximation

In the two-beam approximation, as an elementary example, equation (5.2.6.2) takes the form

$$\begin{pmatrix} u_0 \\ u_{\mathbf{h}} \end{pmatrix} = \exp\left\{i\begin{pmatrix} 0 & V^*(\mathbf{h}) \\ V(\mathbf{h}) & K_{\mathbf{h}} \end{pmatrix}T\right\}\begin{pmatrix} 0 \\ 1 \end{pmatrix}. \qquad (5.2.7.1)$$

If this expression is expanded directly as a Taylor series, it proves surprisingly difficult to sum. However, the symmetries of Clifford algebra can be exploited by summing in a Pauli basis thus,

$$\exp\left\{i\begin{pmatrix} 0 & V^*(\mathbf{h}) \\ V(\mathbf{h}) & K_{\mathbf{h}} \end{pmatrix}T\right\}$$
$$= \exp\left\{i\frac{K_{\mathbf{h}}T}{2}\right\}\mathbf{E}\exp\left\{i\left(\frac{K_{\mathbf{h}}}{2}\boldsymbol{\sigma}_3 + V^R\boldsymbol{\sigma}_1 - V^I\boldsymbol{\sigma}_2\right)T\right\}.$$

Here, the $\boldsymbol{\sigma}_i$ are the Pauli matrices

$$\boldsymbol{\sigma}_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},\ \boldsymbol{\sigma}_3 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$
$$\mathbf{E} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

and V^R, V^I are the real and imaginary parts of the complex scattering coefficients appropriate to a noncentrosymmetric crystal,

references