$$|U\rangle = \exp\{i\mathbf{M}_{\rm p}T\}|0\rangle \qquad (5.2.6.2)$$

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.

$$\mathbf{S} = \exp\{i\mathbf{M}_{\rm p}T\}$$

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,

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

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 $V^{\rm R}$, $V^{\rm I}$ are the real and imaginary parts of the complex scattering coefficients appropriate to a noncentrosymmetric crystal, *i.e.* $V_{\mathbf{h}} = V^{\rm R} + iV^{\rm I}$. Expanding,

$$\begin{aligned}\exp&\left\{i\left(\frac{K_{\mathbf{h}}}{2}\boldsymbol{\sigma}_3 + V^{\rm R}\boldsymbol{\sigma}_1 - V^{\rm I}\boldsymbol{\sigma}_2\right)T\right\}\\ &= \mathbf{E} + i\left(\frac{K_{\mathbf{h}}}{2}\boldsymbol{\sigma}_3 + V^{\rm R}\boldsymbol{\sigma}_1 - V^{\rm I}\boldsymbol{\sigma}_2\right)T\\ &\quad -\frac{1}{2}\left(\frac{K_{\mathbf{h}}}{2}\boldsymbol{\sigma}_3 + V^{\rm R}\boldsymbol{\sigma}_1 - V^{\rm I}\boldsymbol{\sigma}_2\right)^2 T^2 + \ldots,\end{aligned}$$

using the anti-commuting properties of $\boldsymbol{\sigma}_i$:

$$\left.\begin{aligned}\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j\boldsymbol{\sigma}_i &= 0\\ \boldsymbol{\sigma}_i\boldsymbol{\sigma}_i &= 1\end{aligned}\right\}$$

and putting $[(K_{\mathbf{h}}/2)^2 + V(\mathbf{h})V^*(\mathbf{h})] = \Omega$, $\mathbf{M}_2 = [(K_{\mathbf{h}}/2)\boldsymbol{\sigma}_3 + V^{\rm R}\boldsymbol{\sigma}_1 - V^{\rm I}\boldsymbol{\sigma}_2]$, so that $\mathbf{M}_2^2 = \Omega\mathbf{E}$ and $\mathbf{M}_2^3 = \Omega\mathbf{M}_2$, the powers of the matrix can easily be evaluated. They fall into odd and even series, corresponding to sine and cosine, and the classical two-beam approximation is obtained in the form

$$\mathbf{Q}_2 = \exp\{i(K_{\mathbf{h}}/2)T\}\mathbf{E}\left[(\cos\Omega^{1/2}T)\mathbf{E} + i\left(\frac{\sin\Omega^{1/2}T}{\Omega^{1/2}}\right)\mathbf{M}_2\right]. \qquad (5.2.7.2)$$

This result was first obtained by Blackman (1939), using Bethe's dispersion formulation. Ewald and, independently, Darwin, each with different techniques, had, in establishing the theoretical foundations for X-ray diffraction, obtained analogous results (see Section 5.1.3).

The two-beam approximation, despite its simplicity, exemplifies some of the characteristics of the full dynamical theory, for instance in the coupling between beams. As Ewald pointed out, a formal analogy can be found in classical mechanics with the motion of coupled pendulums. In addition, the functional form $(\sin ax)/x$, deriving from the shape function of the crystal emerges, as it does, albeit less obviously, in the N-beam theory.

This derivation of equation (5.2.7.2) exhibits two-beam diffraction as a typical two-level system having analogies with, for instance, lasers and nuclear magnetic resonance and exhibiting the symmetries of the special unitary group SU(2) (Gilmore, 1974).

5.2.8. Eigenvalue approach

In terms of the eigenvalues and eigenvectors, defined by

$$\mathbf{H}_{\rm p}|\,j\rangle = \gamma_j|\,j\rangle,$$

the evolution operator can be written as

$$\mathbf{U}(z, z_0) = \textstyle\int |\,j\rangle\exp\{\gamma_j(z - z_0)\}\langle j|\,{\rm d}j.$$

This integration becomes a summation over discrete eigen states when an infinitely periodic potential is considered.

Despite the early developments by Bethe (1928), an N-beam expression for a transmitted wavefunction in terms of the eigenvalues and eigenvectors of the problem was not obtained until Fujimoto (1959) derived the expression

$$U_{\mathbf{h}} = \sum_j \psi_0^{j*}\psi_{\mathbf{h}}^j\exp\{-i2\pi\gamma_j T\}, \qquad (5.2.8.1)$$

where $\psi_{\mathbf{h}}^j$ is the h component of the j eigenvector with eigenvalue γ_j.

This expression can now be related to those obtained in the other formulations. For example, Sylvester's theorem (Frazer *et al.*, 1963) in the form

$$f(\mathbf{M}) = \sum_j \mathbf{A}_j f(\gamma_j)$$

when applied to Sturkey's solution yields

$$\boldsymbol{\Phi}_{\mathbf{h}} = \exp(i\mathbf{M}_{\rm p}z) = \textstyle\sum \mathbf{P}_j\exp\{i2\pi\gamma_j z\}$$

(Kainuma, 1968; Hurley *et al.*, 1978). Here, the $\mathbf{P}_j$ are projection operators, typically of the form

$$\mathbf{P}_j = \prod_{n\neq j}\frac{(\mathbf{M}_{\rm p} - \mathbf{E}\gamma_n)}{\gamma_j - \gamma_n}.$$