International Tables for Crystallography (2006). Vol. B, Section 5.2.8, p. 554.

i.e. $V_{\mathbf{h}} = V^R + iV^I$. Expanding,

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

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 $[(K_{\mathbf{h}}/2)^2 + V(\mathbf{h})V^*(\mathbf{h})] = \Omega$, $\mathbf{M}_2 = [(K_{\mathbf{h}}/2)\boldsymbol{\sigma}_3 + V^R\boldsymbol{\sigma}_1 - V^I\boldsymbol{\sigma}_2]$, 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

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

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

$$\mathbf{H}_p|\,j\rangle = \gamma_j|\,j\rangle,$$

the evolution operator can be written as

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

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

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

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

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

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

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

On changing to a lattice basis, these transform to $\psi_0^{j*}\psi_{\mathbf{h}}^j$.

Alternatively, the semi-reciprocal differential equation can be uncoupled by diagonalizing $\mathbf{M}_p$ (Goodman & Moodie, 1974), a process which involves the solution of the characteristic equation

$$|\mathbf{M}_p - \gamma_j\mathbf{E}| = 0. \quad (5.2.8.2)$$

5.2.9. Translational invariance

An important result deriving from Bethe's initial analysis, and not made explicit in the preceding formulations, is that the fundamental symmetry of a crystal, namely translational invariance, by itself imposes a specific form on wavefunctions satisfying Schrödinger's equation.

Suppose that, in a one-dimensional description, the potential in a Hamiltonian $\mathbf{H}_t(x)$ is periodic, with period t. Then,

$$\varphi(x + t) = \varphi(x)$$

and

$$\mathbf{H}_t\psi(x) = \mathbf{E}\psi(x).$$

Now define a translation operator

$$\boldsymbol{\Gamma}f(x) = f(x + t),$$

for arbitrary $f(x)$. Then, since $\boldsymbol{\Gamma}\varphi(x) = \varphi(x)$, and ∇^2 is invariant under translation,

$$\boldsymbol{\Gamma}\mathbf{H}_t(x) = \mathbf{H}_t(x)$$

and

$$\boldsymbol{\Gamma}\mathbf{H}_t(x)\psi(x) = \mathbf{H}_t(x + t)\psi(x + t) = \mathbf{H}_t(x)\boldsymbol{\Gamma}\psi(x).$$

Thus, the translation operator and the Hamiltonian commute, and therefore have the same eigenfunctions (but not of course the same eigenvalues), *i.e.*

$$\boldsymbol{\Gamma}\psi(x) = \alpha\psi(x).$$

This is a simpler equation to deal with than that involving the Hamiltonian, since raising the operator to an arbitrary power simply increments the argument

$$\boldsymbol{\Gamma}^m\psi(x) = \psi(x + mt) = \alpha^m\psi(x).$$

But $\psi(x)$ is bounded over the entire range of its argument, positive and negative, so that $|\alpha| = 1$, and α must be of the form $\exp\{i2\pi kt\}$.

Thus, $\psi(x + t) = \boldsymbol{\Gamma}\psi(x) = \exp\{i2\pi kt\}\psi(x)$, for which the solution is

$$\psi(x) = \exp\{i2\pi kt\}q(x)$$

with $q(x + t) = q(x)$.

This is the result derived independently by Bethe and Bloch. Functions of this form constitute bases for the translation group, and are generally known as Bloch functions. When extended in a direct fashion into three dimensions, functions of this form ultimately embody the symmetries of the Bravais lattice; *i.e.* Bloch functions are the irreducible representations of the translational component of the space group.

references