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 $\mathbf{M}_{\rm p}$ (Goodman & Moodie, 1974), a process which involves the solution of the characteristic equation

$$|\mathbf{M}_{\rm p} - \gamma_j \mathbf{E}| = 0. \qquad (5.2.8.2)$$

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

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

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

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

and

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

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

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

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

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

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, $\psi(x+t) = \mathbf{\Gamma}\psi(x) = \exp\{i2\pi kt\}\psi(x)$, 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.

5.2.10. Bloch-wave formulations

In developing the theory from the beginning by eigenvalue techniques, it is usual to invoke the periodicity of the crystal in order to show that the solutions to the wave equation for a given wavevector $\mathbf{k}$ are Bloch waves of the form

$$\psi = C(\mathbf{r})\exp\{i\mathbf{k}\cdot\mathbf{r}\},$$

where $C(\mathbf{r})$ has the periodicity of the lattice, and hence may be expanded in a Fourier series to give

$$\psi = \sum_{\mathbf{h}} C_{\mathbf{h}}(\mathbf{k})\exp\{i(\mathbf{k}+2\pi\mathbf{h})\cdot\mathbf{r}\}. \qquad (5.2.10.1)$$

The $C_{\mathbf{h}}(\mathbf{k})$ are determined by equations of consistency obtained by substitution of equation (5.2.10.1) into the wave equation.

If N terms are selected in equation (5.2.10.1) there will be N Bloch waves where wavevectors differ only in their components normal to the crystal surface, and the total wavefunction will consist of a linear combination of these Bloch waves. The problem is now reduced to the problem of equation (5.2.8.2).

The development of solutions for particular geometries follows that for the X-ray case, Chapter 5.1, with the notable differences that:

(1) The two-beam solution is not adequate except as a first approximation for particular orientations of crystals having small unit cells and for accelerating voltages not greater than about 100 keV. In general, many-beam solutions must be sought.

(2) For transmission HEED, the scattering angles are sufficiently small to allow the use of a small-angle forward-scattering approximation.

(3) Polarization effects are negligible except for very low energy electrons.

Humphreys (1979) compares the action of the crystal, in the Bloch-wave formalism, with that of an interferometer, the incident beam being partitioned into a set of Bloch waves of different wavevectors. 'As each Bloch wave propagates it becomes out of phase with its neighbours (due to its different wavevector). Hence interference occurs. For example, if the crystal thickness varies, interference fringes known as thickness fringes are formed.' For the two-beam case, these are the fringes of the pendulum solution referred to previously.

5.2.11. Dispersion surfaces

One of the important constructs of the Bloch-wave formalism is the dispersion surface, a plot of the permitted values of the z component of a Bloch wavevector against the component of the incident wavevector parallel to the crystal surface. The curve for a particular Bloch wave is called a branch. Thus, for fast electrons, the two-beam approximation has two branches, one for each eigenvalue, and the N-beam approximation has N.

A detailed treatment of the extensive and powerful theory that has grown from Bethe's initial paper is to be found, for example, in Hirsch *et al.* (1965). Apart from its fundamental importance as a theoretical tool, this formulation provides the basis for one of the most commonly used numerical techniques, the essential step being the estimation of the eigenvalues from equation (5.2.8.2) [see *IT* C (2004, Section 4.3.6.2)].