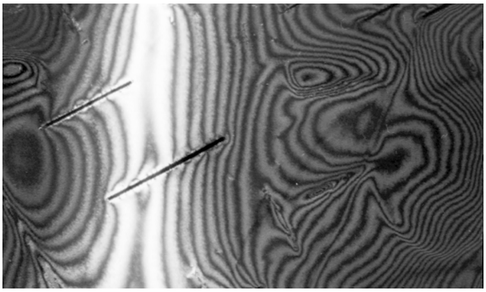
# 12. Dynamical Theory



## 12.1 Chapter Overview

This chapter solves the Schrödinger equation for a high-energy electron in a solid with translational periodicity – i.e., a crystal. Section 12.2.1 derives the dynamical equations (the "Howie–Whelan–Darwin equations") from the Bethe treatment of the Schrödinger equation, and contains the most condensed mathematics in the book. For a first approach to this chapter, the authors recommend reading the following sections in this order: 12.3, the first two short subsections of 11.2.1, 12.2.3, the first subsection of 12.4.1, and finally 12.5. These sections offer an intuitive understanding of the issues in dynamical theory. They show how the wavefunction of the high-energy electron is affected by the potential energy of the crystal – specifically, the periodicity of the potential energy that originates with the periodicity of the atom arrangements. It turns out that the periodic potential causes the amplitude of the high-energy electron to be transferred back-and-forth ("dynamically") between the forward-scattered[1] and diffracted wavefunctions (12.20). At the precise Laue condition for strong diffraction ($s = 0$), the physical distance

---

[1] It is no longer proper to use the term "transmitted beam" as we did for kinematical theory because the beam leaving the sample in the forward direction has undergone many interchanges of energy with the diffracted beams.

over which the wave amplitude is transferred back-and-forth once is called the "extinction distance." The extinction distance is shown to be inversely proportional to the Fourier component of the crystal potential, $U_{\boldsymbol{g}}$, where $\boldsymbol{g}$ equals the difference in wavevector of the two coupled beams.

Quantum mechanics allows an electron wavefunction to be described by different "representations," which employ different sets of orthogonal basis functions. The "beam representation" $\{\Phi(\boldsymbol{g})\}$, and the "Bloch wave representation" $\{\Psi(\boldsymbol{r})\}$, are the two representations used in this chapter. The reader is already familiar with the forward and diffracted wavefunctions $\Phi_0(\boldsymbol{r})$ and $\Phi_{\boldsymbol{g}}(\boldsymbol{r})$ of the beam representation, whose amplitudes, $\phi_0(z)$ and $\phi_{\boldsymbol{g}}(z)$, vary with depth $z$ into the specimen. In its simplest form, the Bloch wave representation uses two Bloch wavefunctions, $\Psi^{(1)}(\boldsymbol{r})$ and $\Psi^{(2)}(\boldsymbol{r})$. It is a convenient representation for an electron that propagates in a crystal because the amplitudes of the Bloch wavefunctions, $\psi^{(1)}$ and $\psi^{(2)}$, are constant throughout a perfect crystal. Bloch waves are eigenfunctions of an infinite, periodic crystal. Although the different Bloch waves have the same total energy, their electron density is distributed differently within the unit cell. The different Bloch waves therefore have slightly different balances between potential energy and kinetic energy. Our two Bloch waves therefore have wavevectors differing slightly from an average $k$ as $k + \gamma^{(1)}$ and $k + \gamma^{(2)}$, and these $\gamma^{(j)}$ increase with the Fourier component of the crystal potential, $U_{\boldsymbol{g}}$. The difference between $\gamma^{(1)}$ and $\gamma^{(2)}$ gives rise to a spatial periodicity, $1/(\gamma^{(1)} - \gamma^{(2)})$, that proves to be the effective extinction distance for transfer of amplitude between the forward and diffracted beams.

On the other hand, the diffracted beams, $\{\Phi(\boldsymbol{g})\}$, are plane wave states for the electron. They have wavevectors of exactly the same magnitude, although different orientations. They are eigenfunctions of the momentum operator, $-\mathrm{i}\hbar\,\mathbf{grad}$, which means they are solutions to the Schrödinger equation for an isotropic and featureless space, i.e., a constant potential. Since a crystal has a periodic potential that is weak compared to an electron energy of 200 keV, for example, the beams $\{\Phi(\boldsymbol{g})\}$ are almost eigenfunctions of the crystal, but they vary in amplitude through the depth of the crystal. The beams prove useful for calculating the electron scattering at the location of a defect such as a stacking fault. The beams are easily related to the eigenstates of the isotropic vacuum below the specimen, so the beam representation is needed again at the exit surface of the sample to send the electron through the imaging lenses of the microscope.

Here is a brief overview of the phenomena and tools of dynamical theory that are presented in this chapter. It is important to be able to switch easily between the Bloch wave representation and the beam representation. Specifically, we need to a means to express the same electron wavefunction in terms of amplitudes of beams or amplitudes of Bloch waves. This transformation is performed with (12.76) and (12.77). The coefficients $\left\{C_{\boldsymbol{g}}^{(j)}\right\}$ for the transformation matrix are given in (12.140) and (12.141). They depend on the extinction distance and on the tilt of the incident beam (parameterized by the deviation parameter, $s$, often called the "diffraction error"). It turns out that the amplitudes of the Bloch waves are easiest to obtain at the top of the specimen, where there is only a forward beam and (12.77) does not depend on the sample thickness (because $z = 0$). A tool to obtain these amplitudes is shown in Fig. 12.17, the "dispersion surface construction," akin to the Ewald sphere construction. It provides a quick indication of how $s$ affects the amplitudes of the Bloch waves.

Dynamical calculations of diffraction contrast are presented later in the chapter. For a perfect crystal of finite size, it is interesting that the diffracted intensity (12.161) has the same mathematical form as the intensity of kinematical theory (7.12). As discussed in Sects. 7.3 and 12.5, however, there are several differences in predictions of diffraction contrast from crystal defects by kinematical and dynamical theories. Hirsch, et al.'s classic example of using Bloch waves and beams for calculating diffraction contrast from stacking faults is presented in Sect. 12.7.2. In spite of the complexity of this dynamical treatment, without a further extension it misses a most important feature of diffraction contrast from stacking faults – the lack of complementary fringe contrast in bright- and dark-field images. This asymmetry of diffraction contrast from the top and bottom of the sample involves the effects of "absorption." As used here, absorption means any incoherent scattering process – the high-energy electron need not disappear, but merely lose coherence. Absorption can be included by adding an imaginary component to the crystal potential. Section 12.7.3 describes the effects of absorption in a qualitative way.

## 12.2 ‡ * Mathematical Features of High-Energy Electrons in a Periodic Potential

### 12.2.1 ‡ * The Schrödinger Equation

**The Average Potential of a Solid.** Before we consider the periodicity of the crystal potential, we consider the effect of the average potential in the solid, denoted $U_{00}$. This potential is electrostatic in origin, and is attractive (i.e., $U_{00} < 0$) because the high-energy electron enters the positive ion cores as it passes through the solid. This potential alters the electron wavevector in the solid, $\boldsymbol{k}$. This wavevector is related to the kinetic energy of the electron in the solid, $E_{\mathrm{kin}}$, in the usual way:

$$\frac{\hbar^2 k^2}{2m} = E_{\mathrm{kin}} \; . \tag{12.1}$$

Conservation of energy is used to find the effect of $U_{00}$ on the electron wavevector. When the electron enters the potential of the solid, its kinetic