International Tables for Crystallography (2012). Vol. F, Figure 2.1.4.1, p. 53.

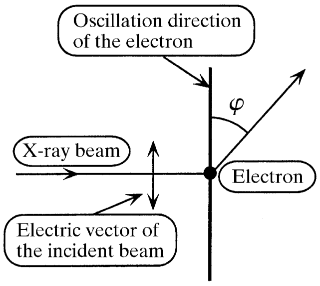

Figure 2.1.4.1
The electric vector of a monochromatic and polarized X-ray beam is in the plane. It hits an electron, which starts to oscillate in the same direction as the electric vector of the beam. The oscillating electron acts as a source of X-rays. The scattered intensity depends on the angle φ between the oscillation direction of the electron and the scattering direction [equation (2.1.4.1)]. Reproduced with permission from Drenth (1999). Copyright (1999) Springer-Verlag.

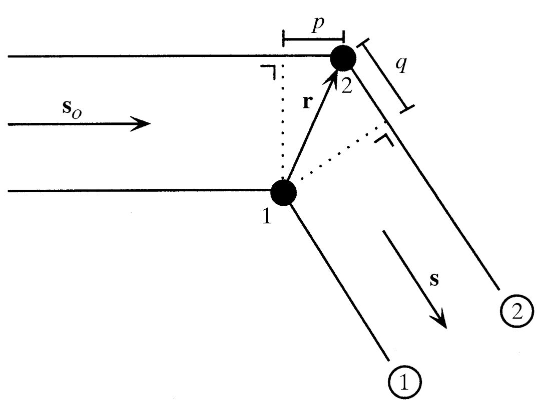

Figure 2.1.4.2
The black dots are electrons. The origin of the system is at electron 1; electron 2 is at position **r**. The electrons are irradiated by an X-ray beam from the direction indicated by vector $\mathbf{s}_o$. The radiation scattered by the electrons is observed in the direction of vector **s**. Because of the path difference $p + q$, scattered beam 2 will lag behind scattered beam 1 in phase. Reproduced with permission from Drenth (1999). Copyright (1999) Springer-Verlag.

radiation, and this is the radiation responsible for the interference effects in diffraction. It was shown by Thomson that if the electron is completely free the following hold:

(1) The phase difference between the incident and the scattered beam is π, because the scattered radiation is proportional to the displacement of the electron, which differs by π in phase with its acceleration imposed by the electric vector.
(2) The amplitude of the electric component of the scattered wave at a distance r which is large in comparison with the wavelength of the radiation is

$$E_{\rm el} = E_o \frac{1}{r}\frac{e^2}{mc^2}\sin\varphi,$$

where E_o is the amplitude of the electric vector of the incident beam, e is the electron charge, m is its mass, c is the speed of light and φ is the angle between the oscillation direction of the electron and the scattering direction (Fig. 2.1.4.1). Note that $E_o \sin\varphi$ is the component of E_o perpendicular to the scattering direction.

In terms of energy,

$$I_{\rm el} = I_o \frac{1}{r^2}\left(\frac{e^2}{mc^2}\right)^2 \sin^2\varphi. \qquad (2.1.4.1a)$$

The scattered energy per unit solid angle is

$$I_{\rm el}(\Omega = 1) = I_{\rm el} r^2. \qquad (2.1.4.1b)$$

It was shown by Klein & Nishina (1929) [see also Heitler (1966)] that the scattering by an electron can be discussed in terms of the classical Thomson scattering if the quantum energy $h\nu \ll mc^2$. This is not true for very short X-ray wavelengths. For $\lambda = 0.0243$ Å, $h\nu$ and mc^2 are exactly equal, but for $\lambda = 1.0$ Å, $h\nu$ is 0.0243 times mc^2. Since wavelengths in macromolecular crystallography are usually in the range 0.8–2.5 Å, the classical approximation is allowed. It should be noted that:

(1) The intensity scattered by a free electron is independent of the wavelength.
(2) Thomson's equation can also be applied to other charged particles, *e.g.* a proton. Because the mass of a proton is 1800 times the electron mass, scattering by protons and by atomic nuclei can be neglected.
(3) Equation (2.1.4.1*a*) gives the scattering for a polarized beam. For an unpolarized beam, $\sin^2\varphi$ is replaced by a suitable polarization factor.

2.1.4.2. *Scattering by a system of two electrons*

This can be derived along classical lines by calculating the phase difference between the X-ray beams scattered by each of the two electrons. A derivation based on quantum mechanics leads exactly to the same result by calculating the transition probability for the scattering of a primary quantum $(h\nu)_o$, given a secondary quantum $h\nu$ (Heitler, 1966, p. 193). For simplification we shall give only the classical derivation here. In Fig. 2.1.4.2, a system of two electrons is drawn with the origin at electron 1 and electron 2 at position **r**. They scatter the incident beam in a direction given by the vector **s**. The direction of the incident beam is along the vector $\mathbf{s}_o$. The length of the vectors can be chosen arbitrarily, but for convenience they are given a length $1/\lambda$. The two electrons scatter completely independently of each other.

Therefore, the amplitudes of the scattered beams 1 and 2 are equal, but they have a phase difference resulting from the path difference between the beam passing through electron 2 and the beam passing through electron 1. The path difference is $p + q = \lambda[\mathbf{r}\cdot(\mathbf{s}_o - \mathbf{s})]$. Beam 2 lags behind in phase compared with beam 1, and with respect to wave 1 its phase angle is

$$-2\pi\lambda[\mathbf{r}\cdot(\mathbf{s}_o - \mathbf{s})]/\lambda = 2\pi\mathbf{r}\cdot\mathbf{S}, \qquad (2.1.4.2)$$

where $\mathbf{S} = \mathbf{s} - \mathbf{s}_o$.

From Fig. 2.1.4.3, it is clear that the direction of **S** is perpendicular to an imaginary plane reflecting the incident beam at an angle θ and that the length of **S** is given by

$$|\mathbf{S}| = 2\sin\theta/\lambda. \qquad (2.1.4.3)$$

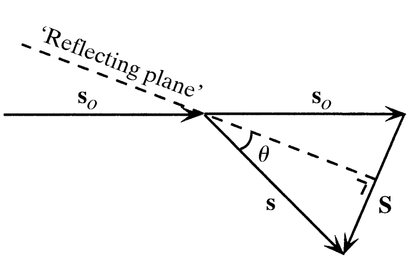

Figure 2.1.4.3
The direction of the incident wave is indicated by $\mathbf{s}_o$ and that of the scattered wave by **s**. Both vectors are of length $1/\lambda$. A plane that makes equal angles with **s** and $\mathbf{s}_o$ can be regarded as a mirror reflecting the incident beam. Reproduced with permission from Drenth (1999). Copyright (1999) Springer-Verlag.

references