

Two kinds of waves: these last big equations are of a form:
 (Amplitude factor) • (Phase factor) Which is just the general equation of a wave.
 However, there are two varieties:

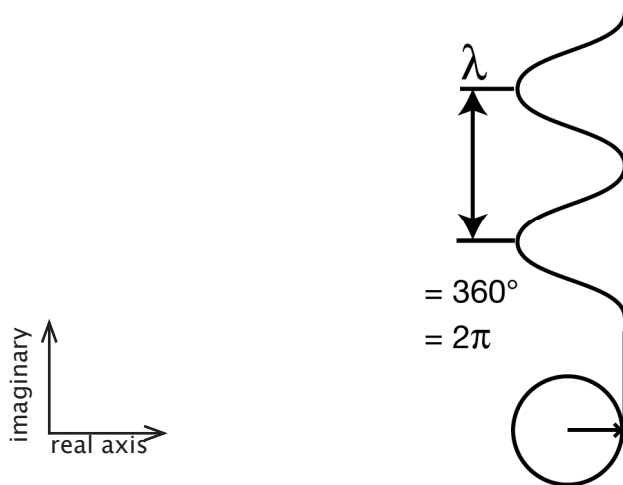
1) $|F_{hkl}| \cdot e^{i\phi_{hkl}}$ the expression for a real x-ray, with a real, experimentally fixed, wavelength.

A resultant diffracted x-ray wave from the crystal is the sum of x-ray waves scattered from each and every atom in that crystal in a particular direction. Each resultant wave, indexed as h, k, l , travels out of the crystal in that particular direction, so we will need to learn how to combine parallel x-ray waves to form a resultant wave.

2) (amplitude factor) • $e^{-i2\pi(hx + ky + \ell z)}$ some other kind of wave, with wavelengths that turn out to be integral fractions of the dimensions of the unit cell.

The electron density in a model of the crystal is the sum of these second kind of waves. Not only are the wavelengths of these density waves different from each other, each wave is going in its own particular direction. The wavelengths are integral fractions of unit cell dimensions (i.e. 1,2,3,... complete cycles within the bounds of the unit cell), thus they are standing waves. So we will need to learn how to combine standing waves in a box (the unit cell) to build up a density-like image.

Representing waves, the phase clock (with radius = amplitude):



ϕ factor ($e^{i\phi}$): exponential form convenient to talk about; $e^{i\phi} = \cos(\phi) + i \sin(\phi)$
 $\cos()$ & $\sin()$ form (real and imaginary components) sometimes more convenient for computation.