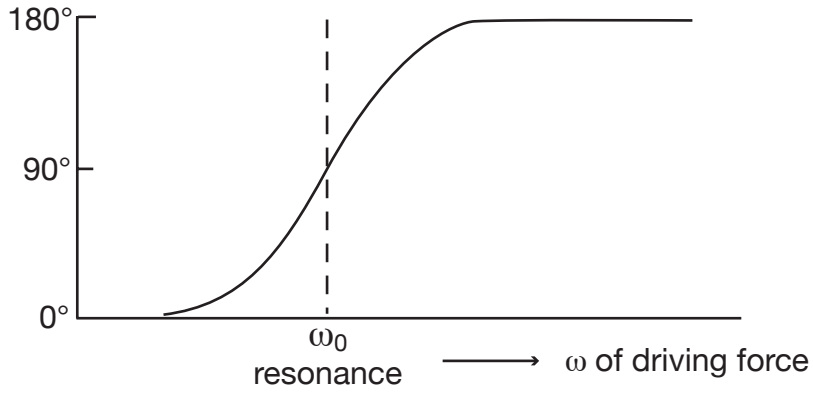
Anomalous Scattering

Usually the x-ray wave which drives the electrons into forced vibrations is of a much higher frequency than the resonant frequency of the electrons. In this case, the forced damped simple harmonic oscillations of the electrons will be 180° out of phase with the driving wave. This behavior is a completely general characteristic of forced simple harmonic motion. It depends on the interaction of the driving force and the natural restoring force of the oscillator, and it can easily be demonstrated with a pendulum or spring. The relationship of phase lag to frequency is shown on the diagram:



Sometimes the binding of some inner electrons of an atom is of such a strength that the resonant frequency is shifted from that usual for free electrons toward the frequency of the x-ray wave. These electrons will oscillate nearer to 90° out of phase (and also more violently, since they are nearer resonance). For a given atom, then, most of the scattered ray has a 180° phase lag and there will be a few electrons-worth of scattering with a 90° phase lag. Relative to the normal diffracted ray, therefore, the anomalous part of the scattering has a 90° phase advance.

The amount of anomalous scattering for a given atomic species is known and can be looked up in tables (International Tables for Crystallography, Vol. III). For a given x-ray wavelength an atom's scattering will be described as:

$$f_{total} = f_0 + f' + if''$$

usual scattering at that 2θ

correction to usual scattering

number electrons-worth of anomalous scattering

means 90° out of phase