Materials 286C/UCSB: Class III — Optical diffraction, Fourier transforms, the generation of X-rays, the Laue and Bragg experiments, Bragg's law

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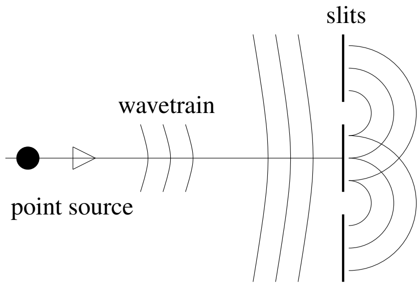
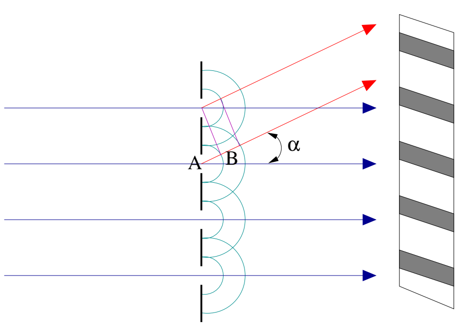
Optical diffraction

Fresnel diffraction



In the Fresnel diffraction experiment, wavetrains from a single point source arrive at two or more slits, through which they pass. The slits act as a secondary light source. As they emerge from the slits, they interfere constructively and destructively, forming dark and light bands.

Fraunhofer diffraction



In Fraunhofer diffraction, a set or parallel rays pass through a number of slits. Constructive and destructive interference occurs as bands on the right hand side. The condition for constructive interference is that the path difference AB, between adjacent slits, should be an integral multiple of the number of wavelengths. If the separation between slits is a, the path difference is:

$$\mathrm{AB} = n\lambda = a\sin\alpha$$

If the image is taken at some far-away location, then α is small and $\sin\alpha \sim \alpha$ and

$$\alpha \sim \frac{n\lambda}{a}$$

a reciprocal relationship between the diffraction angle and the (slit) lattice spacings a.

Fourier transforms

The Fourier transform of the function $f(x)$ is defined:

$$F(k) = \int_{-\infty}^{\infty} f(x) e^{-2\pi ikx} dk$$

and it's inverse is defined:

$$f(x) = \int_{-\infty}^{\infty} F(k) e^{2\pi ikx} dx$$

For even functions $f(x) = f(-x)$ and only the cosine part of the exponent is retained:

$$F(k) = 2\int_{0}^{\infty} f(x) \cos 2\pi kx dk$$

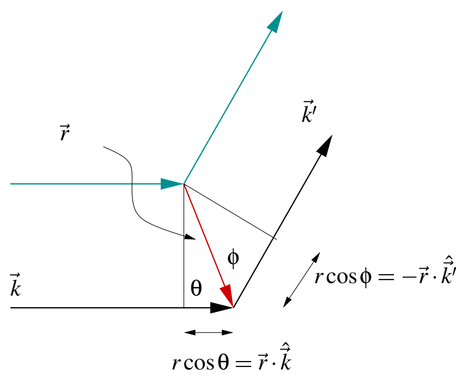
Since the argument of the exponent or the cosine must be dimensionless, the units of k and x are inverses of one-another. So x in Å means k has the units of Å^{-1} which is the units of wavenumber. This is a clue that the Fourier transforms of distances (spacings) should be functions of wavelnumbers.

A particularly useful Fourier transform is that of the cosine:

$f(x)$	$F(k)$
$\cos(2\pi k_0 x)$	$\frac{1}{2}[\delta(k-k_0) + \delta(k+k_0)]$

A periodic function with wavelength (k_0) is transformed to a single spike, corresponding to that wavelength. Lattices are periodic so one expects that their Fourier transforms will possess information about all the spacings in the lattice.

What is the connection between the scattered/diffracted radiation and the Fourier Transform ?



Consider a "pencil" of radiation being scattered from some point p in an object (black arrows). Let the incident vector be $\vec{k}$ and the scattered vector be $\vec{k}'$. Now consider the path difference of the scatterer ed vector, with the same pencil of radiation passing through the origin in the object. This is represented by the green arrows. The vector $\vec{r}$ (red) allows the path difference to be calculated as:

$$r\cos\theta + r\cos\phi = \vec{r}\cdot\hat{\vec{k}} + -\vec{r}\cdot\hat{\vec{k}}'$$

So the path difference is

$$\vec{r} \cdot (\hat{\vec{k}} - \hat{\vec{k'}})$$

Now since the phase difference is the path difference times $2\pi/\lambda$, we have the phase difference:

$$\vec{r} \cdot (\hat{\vec{k}} - \hat{\vec{k'}}) \times 2\pi/\lambda$$

Let $\vec{q} = \lambda(\hat{\vec{k}} - \hat{\vec{k'}})$. Then the phase difference is $2\pi\vec{r} \cdot \vec{q}$. The corresponding wave is then $\exp(2\pi i\vec{r} \cdot \vec{q})$. Now if we integrate over all points in the object, and $f(\vec{r})$ represents the amplitude of the scattering at the point described by $\vec{r}$, then the total scattering is

$$F(\vec{q}) = \int_{-\infty}^{\infty} f(\vec{r}) e^{(2\pi i\vec{r} \cdot \vec{q})} d\vec{r}$$

Which is nothing but the Fourier transform

The generation of X-rays

Electrons from a glowing filament (usually tungsten or rhenium) are accelerated by applying a DC field (typically of about 30-40 kV). These accelerated electrons are then bombarded against a cooled metal target (Fe, Cu, Mo ...). The electrons slow down when they enter the metal, so they loose energy. This lost energy is emitted as a continuous radiation called *brehmsstrahlung* radiation, usually in the X-ray region of the electromagnetic spectrum (with energies of the order of kV). In addition to the broad *brehmsstrahlung* radiation, there are the so-called *characteristic* X-ray peaks associated with electronic transitions in the target material. These characteristic X-radiations have a much larger intensity than does the *brehmsstrahlung*. The energies of the characteristic radiation depends on which atomic shell of the target material is being excited by the incident electrons (K, L *etc*), as well as the atomic number of the target. The energy of the characteristic radiation is proportional to the atomic number raised to the fourth power.

In lab X-ray diffraction experiments, characteristic radiation from the K shell of Cu (with a wavelength around 1.5 Å) or from the K shell of Mo (with a wavelength around 0.7 Å) is typically used.

When charged particles are accelerated, they release energy continuously. In a synchrotron source, electrons are typically accelerated around a storage ring through the use of magnetic fields. The accelerated electrons emit X-rays when they are sufficiently energized. This X-radiation covers a broad spectrum of wavelengths and is very useful for a number of scattering experiments for which lab X-rays are not suited.

The Laue experiment

In the Laue experiment, the crystal is viewed as a 3D diffraction grating. Vector analysis can be used to determine the path difference in the scattered radiation induced by the crystal lattice. The analysis is similar to our demonstration that the scattering corresponds to a Fourier transform. See the handout.

The Bragg experiment and Bragg's law

Bragg simplified the Laue picture by saying that planes (constituted of atoms) can be assumed to act like mirrors and that the X-rays undergo specular reflection by these mirrors. The path difference between the reflected rays from adjacent mirrors gives rise to constructive and destructive interference. See the handout.