Tue. Oct 29, 2013: elastic light scattering

Properties of light, how light interacts with matter, and how light interacts with itself.
Reference material: "Elastic Scattering" web **Notes** on kinemage website:
http://kinemage.biochem.duke.edu/teaching/BCH681/2013BCH681/

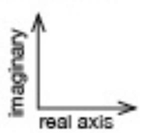
There are 2 really important equations concerning elastic light scattering:
1) Bragg equation: fundamental relationship of distance and direction.
We'll try to get a good feel for these relationships... [Mathematica Bragg Equation Tool, version 20131028]

2) General scattering equation: basis of all analyses ... form is Fourier Transform, very powerful!
We'll introduce this as an outgrowth of our Bragg equation work, and show what the terms and factors mean for understanding scattering by molecules.
Special case 2D general equation diagram (Bragg relationship as we've drawn it on the page plane)
General case 2D
General case 3D using components of 3D vectors

Equation 1

$$n\lambda = 2d\sin(\theta)$$

Bragg relationship shows the smallest scattering angle, 2θ, for the full distance d between scattering points.



$$|F_{C+D}|e^{i\phi_{C+D}} = \mathbf{F}_{C+D} = |F_C|e^{i\phi_C} + |F_D|e^{i\phi_D}$$

Wave amplitudes and phases add as vectors in the complex plane. φ factor ($e^{i\varphi}$); $e^{i\varphi} = \cos(\varphi) + i\sin(\varphi)$

Only can measure Intensity = (resultant amplitude)^2 , but NOT the phase!
(Phase can be deduced from effect of a reference wave on the intensity of the combined wave.)
So what we observe from a scattering experiment is actually in Patterson space - so called because A.L.Patterson figured out the meaning behind the intensity profiles everybody was measuring.
(OK, I'm being provincial, Patterson was a general scattering physicist, but it is the crystallographers who really do use both "real space" and "Patterson space"!

Equation 2

A light wave ray diffracted from a molecule in a crystal (i.e. molecule fixed in space):

A wave is defined by an Amplitude $|F_{hk\ell}|$ and a Phase: $e^{i\phi_{hk\ell}}$

Each diffracted "wave" is a sum of contributions from ALL atoms:

Σ (Amplitude-factors) (Phase-factor) ...the sum is over all atoms.

Amplitude-factors are a property of the atom, including uncertainty about its position.
(Uncertainties are put into the B-factor. Many people think they understand the B-factor because they remember hearing about the Temperature Factor from Physics, for macromolecules the temperature part of the B-factor is only a minor part, most of the effect comes from other kinds of disorder.)

Phase-factor is just dependent on the position of the atom.

Amplitude Phase = (Amplitude-factors) • (Phase-factor)

$$\mathbf{F}_{hk\ell} = |F_{hk\ell}| \cdot e^{i\phi_{hk\ell}} = \sum_{n}^{N} O_n \cdot f_{n,\theta_{hk\ell}} \cdot e^{-B_n (\sin\theta_{hk\ell}/\lambda)^2} \cdot e^{i2\pi(hx_n + ky_n + \ell z_n)}$$

h, k, ℓ : integer index numbers of a particular Bragg Plane, a diffracted ray, a "reflection".

$\theta_{hk\ell}$: angle of incident beam to the h, k, ℓ Bragg plane

$|F_{hk\ell}|$: amplitude of the $hk\ell^{th}$ diffracted ray

$\phi_{hk\ell}$: the phase of the $hk\ell^{th}$ diffracted ray

B : B-factor (historically the Temperature Factor, but dominated by other uncertainties)

$f_{n,\theta_{hk\ell}}$: individual atomic scattering factor of the n^{th} atom as a function of $\theta_{hk\ell}$

x_n, y_n, z_n : coordinates of the n^{th} atom

N : total number of atoms in the repeating unit of the crystal

O_n : occupancy of the n^{th} atom. (e.g. for a half-occupied ligand, sidechain alternate rotamer, etc.)

... many forms of Equation 2 ...

$$|F_{hk\ell}|\, e^{i\phi_{hk\ell}} = \sum_{n=1}^{N} f_n\, e^{i\phi_n}$$

$$|F_{hk\ell}|\, e^{i\phi_{hk\ell}} = \sum_{n=1}^{N} f_n\, e^{i\,2\pi(hx_n + ky_n + \ell z_n)}$$

$$F_{hk\ell}\, e^{i\,\phi_{hk\ell}} = \sum_x \sum_y \sum_z \rho_{xyz}\, e^{i2\pi(hx + ky + \ell z)}$$

equation of a wave

$$\rho_{xyz} = \sum_h \sum_k \sum_\ell F_{hk\ell}\, e^{i\phi_{hk\ell}}\, e^{-i2\pi(hx + ky + \ell z)}$$

$$P_{xyz} = \sum_h \sum_k \sum_\ell |F_{hk\ell}|^2\, e^{-i\,2\pi(hx + ky + \ell z)}$$