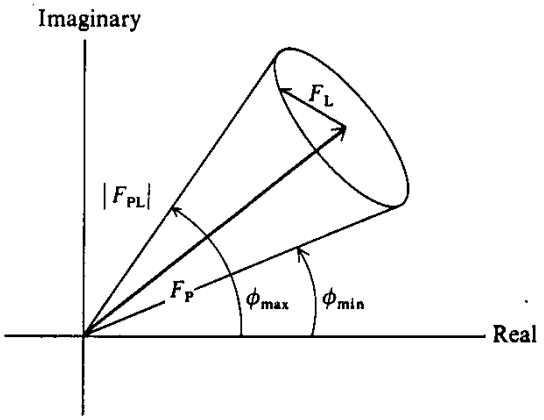
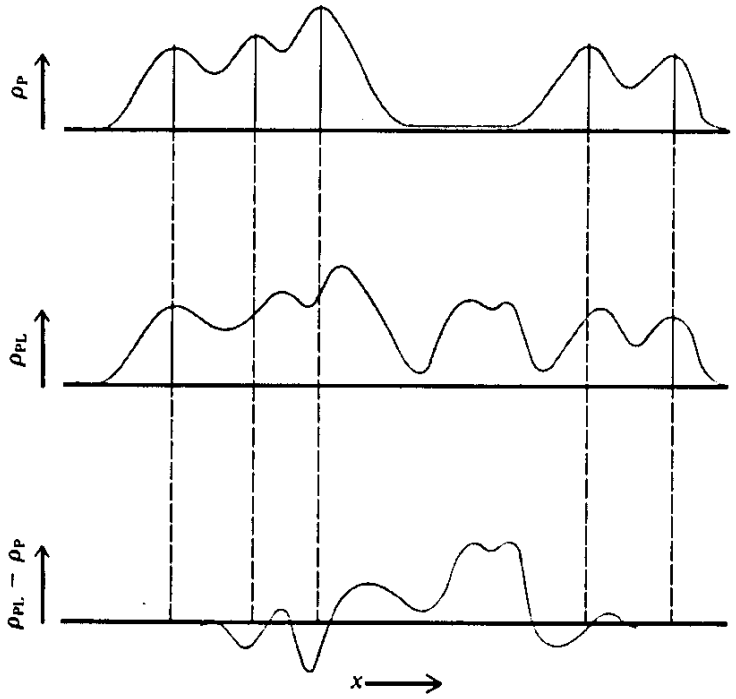


Effect on observed structure factors of an added ligand. The parent-crystal structure factor F_P is presumed to be known. Then, so long as the ligand structure factor $|F_L|$ is small, the phase of F_P is a good approximation of the phase of the ligand complex, F_{PL}.

A difference Fourier map thus can be calculated by :

$$\Delta\rho(x, y, z) = (1/V) \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} [|F_{PL}(h, k, l)| - |F_P(h, k, l)|] e^{i\phi_P(h,k,l)} e^{-2\pi i(hx+ky+lz)}$$



Using difference Fourier syntheses to study ligand binding. Such syntheses can be used to identify ligand binding sites and any conformational changes that accompany addition of the ligand. Shown are one-dimensional schematic drawings of the parent electron density map (ρ_P), the map that would be computed by solving the structure of the ligand complex (ρ_{PL}), and a difference Fourier ($\rho_{PL} - \rho_P$) that could be calculated in a relatively simple fashion (see text). Note that ligand atoms simply lead to increased density, whereas atom movements yield adjacent peaks and troughs in the difference Fourier. [After T. L. Blundell and L. N. Johnson, *Protein Crystallography* (London: Academic Press, 1976).]