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A new derivation of the Fourier transform of a helical structure

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Auszug

Die Theorie der Fourier-Transformierung einer Wendelstruktur wird, bezogen auf die Wendel-Parameter n = Anzahl der Struktur-Einheiten je Umdrehung und h = Höhe der Einheit, entwickelt. Die Theorie bedarf nicht der Translationsperiode c längs der Wendelachse und ist daher gültig sowohl für rationale als auch für irrationale Wendeln. Die Lagen der Schichtlinien in Beugungsdiagrammen können durch die Größen n, h und einen zusätzlichen Parameter q, den Bessel-Index, vollständig wiedergegeben werden; q bestimmt die Ordnung der in der Gleichung für die Strukturamplitude erscheinenden Bessel-Funktion J_q. Die endgültige Formel ist identisch mit der 1960 von RAMACHANDRAN aus der bekannten Gleichung von COCHRAN, CRICK und VAND (1952) abgeleiteten Formel.

Abstract

The theory of the Fourier transform of a helical structure has been worked out in terms of the elementary parameters n (number of units per turn) and h (unit height) which define the helical conformation of the helix. The theory does not require the definition of a translational repeat c along the helical axis, and therefore is equally valid for both rational and irrational helices. The positions of the layer lines in the diffraction pattern can be specified completely in terms of n and h, and in addition, a parameter q, called the Bessel index, which defines the order of the Bessel function J_q which occurs in the formula of the structure amplitude. The final formula is identical with that deduced by RAMACHANDRAN (1960) from the well-known formula of COCHRAN, CRICK and VAND (1952).

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Introduction

The theory of x-ray diffraction by biological fibres is of great importance in molecular biophysics. Since most of the well-oriented fibres show a helical structure, this theory essentially deals with the x-ray scattering by helical structures. The Fourier transform of a helical structure was first calculated by COCHRAN, CRICK and VAND (1952), which was followed by other treatments of varying approach and generality (CRICK, 1953*a*,*b*; KLUG, CRICK and WYCKOFF, 1958; LANG, 1956). In all these derivations, it is assumed that the helix has, in addition to the helical symmetry, also a translational repeat c along the helical axis, i.e. that there exist two integers p and q such that the helix contains p monomer units for every q turns. Although it was indicated even by COCHRAN *et al.* (1952) that a non-rational value is possible for p/q, an approach to the interpretation of the diffraction pattern, which does not require the definition of the repeat c, was first given by RAMACHANDRAN (1960). He showed that the positions of the various layer lines are connected in a simple way to the basic helical elements of the repeating unit (for example, the peptide unit in an α helix), namely h, the height per unit along the helix axis, and n, the number of units per turn of the helix, which may be either rational or irrational. Denoting $1/n$ by t, termed unit twist, and $1/h$ by Z_0, the reciprocal spacing along the helical axis, if $Z = 1/l$, is the reciprocal length corresponding to a layer line of spacing l, then the formula for Z was shown to be

$$Z = (m \pm qt)\, Z_0, \tag{1}$$

where m, q are integers. Here, t may be either rational, or irrational. However, in obtaining this formula for the case of an *irrational* helix, RAMACHANDRAN (1960) derived it as the limit of the rational approximations obtainable from the theory of COCHRAN *et al.* (1952). Such an irrational helix would, however, actually correspond to an infinite translational repeat. Actually, in the helical structure of a biopolymer, the geometry of the structure is defined essentially by the *local* elements h and t, rather than by the large repeat spacing c. It would therefore be desirable to have a theory in terms of the geometrical relationships between neighbouring units in the helical structure. Such a theory of the Fourier transform of a single helix is given below, which is equally valid for rational and irrational values of n. The extension to coiled coils and multiple helices is obvious and is therefore not discussed here.

Fourier transform of an irrational helix

Consider the case when there is only one atom in the helical monomer unit. Let the cylindrical polar coordinates of the atom in the first unit be r_0, ϕ_0, z_0. Then from the geometry of the helix, the coordinates of the atom in the $(k+1)$th unit are given by

$$r_k = r_0; \quad \phi_k = \phi_0 + 2\pi kt; \quad z_k = z_0 + kh, \tag{2}$$

where h is the unit height and t is the unit twist, in fraction of a full turn. The pitch P of the helix is then given by $P = h/t = nh$, n being the number of monomer units per turn.

Let vectors $\mathbf{r}_k$ and $\mathbf{R}$ denote the position vector of the kth atom and the diffraction vector in the reciprocal space respectively. The cylindrical polar components of these vectors may be given by $\mathbf{r}_k = (r_k, \phi_k, z_k)$ and $\mathbf{R} = (R, \Phi, Z)$. The scattering amplitude F_k corresponding to the $(k+1)$th unit is given by

$$\begin{aligned} F_k &= f \exp 2\pi i(\mathbf{R} \cdot \mathbf{r}_k), \\ &= f \exp 2\pi i Rr_0 \cos(\phi_0 + 2\pi kt - \Phi) \exp 2\pi i Z(z_0 + kh), \end{aligned} \tag{3}$$

where f is the scattering factor of the atom in the monomer unit. Noting that $\exp(i\alpha\cos\theta)$ is the generating function of the Bessel functions $J_q(\alpha)$ of integral order, the structure amplitude may be written as

$$F_k = f \exp 2\pi i Z(z_0 + kh) \sum_{q=-\infty}^{+\infty} J_q(2\pi Rr_0) \cdot \exp iq\left(\frac{\pi}{2} + \Phi - \phi_0 - 2\pi kt\right). \tag{4}$$

The total scattering amplitude for the entire helix is obtained by summing the individual scattering amplitudes F_k over all k from $-\infty$ to $+\infty$. Thus,

$$F = \sum_{-\infty}^{+\infty} F_k = \sum_{k=-\infty}^{+\infty} f \exp 2\pi i Z(z_0 + kh) \sum_{q=-\infty}^{+\infty} J_q(2\pi Rr_0) \cdot \exp iq\left(\frac{\pi}{2} + \Phi - \phi_0 - 2\pi kt\right). \tag{5}$$

Separating the quantities that depend only on k and interchanging the sequence of the two summations, we have

$$F = f \sum_{q=-\infty}^{+\infty} J_q(2\pi Rr_0) \cdot \exp\left[2\pi Zz_0 + q\left(\frac{\pi}{2} + \Phi - \phi_0\right)\right] \sum_{k=-\infty}^{+\infty} \exp 2\pi ik(Zh - qt). \tag{6}$$

The second summation is independent of the positional parameters of the atoms in the helix, but involves only the helical parameters h and t. This clearly gives the quantity analogous to the "lattice sum" in standard crystallography.

The value of an infinite sum of the exponentials of the form $\sum_{k=-\infty}^{+\infty} \exp(2\pi i k\alpha)$ may be shown to be non-zero only for integral values of α. Therefore, the lattice sum will have a non-zero value only if $(Zh - qt)$ is equal to an integer, say, m. Thus the condition for non-zero amplitude may be given by the equation

$$Zh - qt = m. \tag{7}$$

With this condition for non-zero scattering amplitude, effected by the lattice sum itself, the value of Z corresponding to these non-zero values of F are given by the equation

$$Z = m/h + qt/h \tag{8}$$

or, in terms of the pitch P of the helix,

$$Z = m(1/h) + q(1/P) \tag{9}$$

where m and q are integers that have values from $-\infty$ to $+\infty$. Eq. (9) gives the locations of the different layer lines that occur, corresponding to various m, q. For a given m and q, the amplitude scattered will be given by

$$F(Z,\Phi,R) = f J_q(2\pi R r_0) \exp i\left[2\pi Z z_0 + q\left(\frac{\pi}{2} + \Phi - \phi_0\right)\right],$$

which gives the variation of F with R on this layer line of reciprocal spacing Z. If, now, the monomer unit consists of more than one atom, then the total scattering amplitude is obtained by summing the above expression over the entire monomer unit. In this case the scattering amplitude becomes

$$F(Z,R,\Phi) = \sum_{j=1}^{N} f_j J_q(2\pi R r_{0j}) \exp i\left[2\pi Z z_{0j} + q\left(\frac{\pi}{2} + \Phi - \phi_{0j}\right)\right], \tag{10}$$

where f_j is the scattering factor of the jth atom in the unit and r_{0j}, ϕ_{0j}, z_{0j} are the coordinates of the jth atom in the first unit, while N is the total number of atoms in the unit. It may be noted that it is possible to sum over the contents of the monomer unit *after* summing over the "lattice", because of the fact that the "lattice sum" does not depend upon the coordinates of the corresponding atom in the first unit, but depends only on the helical parameters.

Discussion

The condition for non-zero amplitude, which leads to Eq. (9), may now be written in terms of $Z_0 (= 1/h)$. Since $(1/P)/(1/h) = h/P = 1/n = t$, we have

$$Z = (m \pm qt) Z_0 , \tag{11}$$

in which m can take all integral values, while $q = 0$ or a positive integer. For a given helix, Z_0 is a constant and hence the above condition gives rise to *layer lines* in the x-ray photograph, whose spacings are related to $h(=1/Z_0)$ by the factor $(m \pm qt)$.

It may be seen that Eq. (10) is exactly identical with that derived for the total scattering amplitude by COCHRAN *et al.* (1952), in which it is seen that the "Bessel index" q of the layer line plays a vital role. However, the height of the layer lines are directly related to the helical parameters (Eq. 11). The x-ray reflections can thus be "indexed" in terms of the integers m and q, without invoking any translational repeat along the helical axis. Thus, the analysis of the x-ray pattern can be completely carried out in terms of the helical parameters n and h, which completely define the geometry of the helix. It may be noticed that, if there are fluctuations in the helical parameters, the indices m and q of a layer line are unaltered, and the variations in the Z values of the different layer lines are only due to the changes in n and h, and these may be calculated by means of Eq. (11).

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References

W. COCHRAN, F. H. C. CRICK and V. VAND (1952), The structure of synthetic polypeptides. I. The transform of atoms on a helix. Acta Crystallogr. **5**, 581–586.

F. H. C. CRICK (1953*a*), The Fourier transform of a coiled-coil. Acta Crystallogr. **6**, 685–689.

F. H. C. CRICK (1953*b*). The packing of α-helices: Simple coiled coils. Acta Crystallogr. **6**, 689–697.

A. KLUG, F. H. C. CRICK and H. W. WYCKOFF (1958), Diffraction by helical structures. Acta Crystallogr. **11**, 199–213.

A. R. LANG (1956), An x-ray study of α-keratin. I. A general diffraction theory for convoluted chain structures and an approximate theory for coiled-coils. Acta Crystallogr. **9**, 436–445.

G. N. RAMACHANDRAN (1960), Analysis of the x-ray diffraction pattern of helical structures. Proc. Indian Acad. Sci. A **52**, 240–254.