possibilités s'offrent aux familles spéciales. Ou bien, chaque position est monocolorée et la famille en question se divise en deux ensembles égaux portant l'un la couleur C_1, l'autre la couleur C_2 [exemple: famille *e* de *p2mm–p2mm* (0, 0, 2, 0, 0, 1)]. Ou bien, toutes les positions de la famille spéciale portent les deux couleurs C_1C_2 [exemple: famille *h* de *p2mm–p2mm* (0, 0, 2, 0, 0, 1)]. Quant aux groupes tricolorés, trois cas se présentent. Dans une famille de positions monocolorées, on rencontre trois ensembles égaux portant respectivement la couleur C_1, C_2 ou C_3 [exemple: famille *a* de *p6–p6* (0, 0, 2, 1, −1, 1)]. Ou bien une famille de positions bicolorées se divise en trois ensembles portant respectivement les deux couleurs C_1C_2, C_1C_3 ou C_2C_3 [exemple: famille *c* de *p6–p6* (0, 0, 2, 1, −1, 1)]. Ou encore les positions de la famille spéciale portent toutes les trois couleurs $C_1C_2C_3$ [exemple: famille *b* de *p6–p6* (0, 0, 2, 1, −1, 1)].

Nous tenons à la disposition du lecteur intéressé les résultats de l'étude complète du coloriage des positions équivalentes générales et spéciales des 184 classes de groupes quadricolorés bidimensionnels.

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Discrete Hilbert Transforms in Crystallography

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Abstract

Under the assumption that the structure amplitude of X-ray diffraction from a crystal satisfies the causal Fourier transform condition and appears to be a function with a band-limited spectrum, discrete Hilbert transforms (DHT) linking structure amplitudes having half-integral-valued Miller indices with structure amplitudes having integral-valued indices are obtained. DHT are then used to derive an interpolation formula that permits structure-amplitude reconstruction from samples with half the sampling frequency of the Nyquist rate. Some one-dimensional test calculations are also given.

Hilbert transforms (HT), or dispersion relations, are well known and widely used in optics (Loudon, 1973), in particle scattering (Hilgevoord, 1960), in electron optics (Misell, Burge & Greenaway, 1974; Saxton, 1974) and in other fields. Considerable theoretical work has been performed with the aim of extracting phase information directly from intensity data with the help of HT (Burge, Fiddy, Greenaway & Ross, 1974, 1976; Taylor, 1981). There have been only a few attempts to apply HT to solve phases in X-ray crystal structure analysis (Ramachandran, 1969; Kaufmann, 1985; Tang & Chang, 1990).

Ramachandran (1969) was the first to pay attention to the possibility of HT application in crystallography. He derived equations similar to HT by differentiating a structure-amplitude expression with respect to the reciprocal-lattice vector. However, the presence of unknown derivatives in Ramachandran's equations was an obstacle to their practical use. Kaufmann (1985) analysed the problem of extracting phase information from intensity measurements by means of HT for X-ray diffraction from crystals and pointed out the difficulties. Tang & Chang (1990) used HT for phase determination in the case of three-beam diffraction.

In this communication an attempt is made to obtain a new expression for DHT by direct discretization of the integral Hilbert transforms.

It is well known that, if a complex function of a real variable $f(x)$ has a Fourier transform $F(y)$ that vanishes for negative argument (causal Fourier transform), $f(x)$ satisfies the Hilbert transform (Toll, 1956; Wu & Ohmura, 1962)

$$f(x) = (1/\pi j) P \int_{-\infty}^{\infty} f(y)/(y-x)\,dy, \qquad (1)$$

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where P denotes the Gauchy principal value; $j = (-1)^{1/2}$. We may write an expression for a structure amplitude in one dimension in the form

$$F(s/a) = \int_0^a \rho(x) \exp[2\pi j(sx/a)]\,dx$$
$$= (1/2\pi) \int_0^{2\pi a} \rho(x') \exp[j(s/a)x']\,dx'. \quad (2)$$

From (2) one can state that the structure amplitude satisfies the causal Fourier transform condition and appears to be a function with a band-limited spectrum and can therefore be expressed in the form of Shannon's sampling theorem (Shannon, 1949; Sayre, 1952; Bricogne, 1974)

$$F(s/a) = \sum_{k=-\infty}^{\infty} F(k/2a)[\sin \pi(2s-k)]/\pi(2s-k), \quad (3)$$

which includes structure amplitudes with both integral and half-integral indices. It should be noted that one can define $F(s/a)$ by the integral over $(-a/2, a/2)$ resulting in the sampling theorem with integral sampling points only (crystallographic sampling). However, in this case, $F(s/a)$ does not satisfy the condition of the causal Fourier transform [$\rho(x)$ must vanish for negative arguments] and cannot be used in Hilbert transforms. So, the use of twice the crystallographic sampling rate in this problem is connected with the applicability of Hilbert transforms to the structure amplitude. It is also important to recall that these two definitions result in different values of $F(s/a)$ only if s does not assume integral values.

It is also known (Papoulis, 1968; Kramer, 1973) that the Hilbert transform of the function

$$f(s) = [\sin \pi(2s-k)]/\pi(2s-k) \quad (4)$$

is

$$\hat{f}(s) = -[1-\cos \pi(2s-k)]/\pi(2s-k). \quad (5)$$

Substitution of (3) into (1) with (4) and (5) taken into account leads to

$$F(s/a) = -(1/j) \sum_{k=-\infty}^{\infty} F(k/2a) \times [1-\cos \pi(2s-k)]/\pi(2s-k). \quad (6)$$

In fact, (6) also provides a series of samples; however, unlike (3), the former allows one to set up linear equations for structure amplitudes.

If one equates the right-hand sides of (3) and (6), one obtains

$$\sum_{k=-\infty}^{\infty} F(k/2a)\{[\sin \pi(2s-k)]/\pi(2s-k) - j[1-\cos \pi(2s-k)]/\pi(2s-k)\} = 0, \quad (7)$$

which holds for any s and shows that the structure amplitudes $F(k/2a)$ are linearly dependent.

Now, by setting $s = h/2$ in (6) or (7) and dividing real and imaginary parts, we get the pair of DHTs

$$A(h/2a) = -(1/\pi) \sum_{k=-\infty}^{\infty}{}' B(k/2a) \times [1-(-1)^{h-k}]/(h-k), \quad (8a)$$

$$B(h/2a) = (1/\pi) \sum_{k=-\infty}^{\infty}{}' A(k/2a) \times [1-(-1)^{h-k}]/(h-k), \quad (8b)$$

where the prime on the summation signs indicates that the terms $h = k$ are omitted. It is clear in (8a) and (8b) that if h is odd only terms with k even will remain and, *vice versa*, for h even only terms with k odd will remain. Thus, DHTs relate structure amplitudes with half-integral indices to structure amplitudes with integral indices and *vice versa*.

It is clear that the DHTs (8a) and (8b) are valid for structure amplitudes from any arbitrary scatterer, *i.e.* for any content of the unit cell. However, if $F(0)$ and the phase of one structure amplitude (fixing the origin) are given with a known magnitude, (8a) and (8b) will represent a set of linear equations with at least as many equations as the unknowns $A(h/a)$, $B(h/a)$, $A(h/2a)$ and $B(h/2a)$. Another system of linear equations for the same unknowns can be set up from (7) and can be solved for s, arbitrarily different from integral values. Unfortunately, the matrices of these problems are weakly conditioned and their solution along the lines of Main & Woolfson (1963) requires additional investigation.

Now let us consider one more possible application of DHT, which could be of interest in the molecular-replacement method and in the analysis of non-crystallographic symmetry (Main & Rossmann, 1966; Crowther, 1969; Colman, 1974; Bricogne, 1974). The interpolation formula (3) includes the samples of the function at the integral as well as the half-integral sampling points. The latter can be evaluated from DHT. Substitution of (8a) into (3) and simple transformations lead to

$$F(s/a) = \sum_{h=-\infty}^{\infty} F\left(\frac{h}{a}\right)\left\{\frac{\sin 2\pi(s-h)}{2\pi(s-h)} + \frac{2j}{\pi^2} \sum_{p=-\infty}^{\infty} \frac{\sin \pi(2s-2p+1)}{(2p-2h-1)(2s-2p+1)}\right\}. \quad (9)$$

Thus the interpolation formula (9) allows one to reconstruct the function [defined in accordance with (2)] from samples with half the sampling frequency of the associated Nyquist rate (Jerri, 1977).

The formulae obtained can be readily extended to three dimensions. Thus, by starting with a

Table 1. *Comparison of left-hand sides and right-hand sides of (8a) and (8b) for a model structure*

$s=h/2$	$A(s)$	$A(s)$ from DHT	$B(s)$	$B(s)$ from DHT
0.0	60.0	59.973	0.0	0.0
0.5	−3.993	−3.991	36.871	36.871
1.0	4.291	4.289	−2.631	−2.631
1.5	−1.879	−1.876	18.056	18.057
2.0	−1.515	−1.517	−4.139	−4.139
2.5	3.431	3.434	10.652	10.652
3.0	−0.921	−0.924	2.070	2.070
3.5	0.487	0.489	10.946	10.947
4.0	−5.047	−5.050	5.426	5.426
4.5	−8.760	−8.757	8.560	8.560
5.0	−9.920	−9.922	−4.990	−4.991
12.5	7.843	7.845	−7.841	−7.840
13.0	−7.371	−7.373	−1.650	−1.651
13.5	10.730	10.732	−16.204	−16.203
14.0	9.057	9.055	6.356	6.355
20.0	−0.533	−0.534	−0.733	−0.734
20.5	−1.801	−1.799	−0.627	−0.626
21.0	0.861	0.859	−1.900	−1.901
21.5	0.599	0.601	0.512	0.513
22.0	0.536	0.534	−0.063	−0.064

Table 2. *Test of (9) for a model structure*

s	$A(s)$	$A(s)$ from (9)	$B(s)$	$B(s)$ from (9)
0.3	27.6592	27.6608	42.9579	42.9568
1.3	10.1056	10.1072	14.0630	14.0619
2.3	8.0863	8.0879	4.4902	4.4891
3.3	3.9060	3.9077	6.7890	6.7879
4.3	−4.3299	−4.3282	7.7530	7.7520
5.3	−2.7180	−2.7164	−3.4647	−3.4657
6.3	5.0526	5.0543	−7.6508	−7.6518
7.3	−4.5736	−4.5719	2.4245	2.4236
8.3	13.5335	13.5353	1.4546	1.4537
9.3	−19.1247	−19.1231	−1.8595	−1.8603
10.3	4.2375	4.2392	−3.0892	−3.0900
20.3	−1.1288	−1.1271	0.1391	0.1387
21.3	1.3511	1.3528	−0.0441	−0.0445
22.3	0.8182	0.8199	0.7965	0.7961
23.3	−1.3696	−1.3679	0.3688	0.3685
24.3	−2.3640	−2.3623	−1.2338	−1.2341
25.3	1.4642	1.4658	2.3129	2.3126
26.3	0.5826	0.5842	−0.7664	−0.7666
27.3	0.9928	0.9944	−1.1980	−1.1982
28.3	0.9265	0.9281	−0.4690	−0.4691

three-dimensional sampling theorem (Petersen & Middleton, 1962) and applying transform (1) to each variable, one can obtain a three-dimensional form of (6),

$$F\left(\frac{s_1}{a_1},\frac{s_2}{a_2},\frac{s_3}{a_3}\right)=-\left(\frac{j}{\pi^2}\right)\sum_{k_1}\sum_{\substack{k_2\\-\infty}}^{\infty}\sum_{k_3}F\left(\frac{k_1}{2a_1},\frac{k_2}{2a_2},\frac{k_3}{2a_3}\right)$$
$$\times\prod_{i=1}^{3}\frac{[1-\cos\pi(2s_i-k_i)]}{\pi(2s_i-k_i)}.$$

Some numerical one-dimensional test calculations were carried out. Tables 1 and 2 show the values of the real and imaginary parts of the structure amplitudes calculated both directly and by use of (8) and (9) for the model structure with ten Gaussian atoms [$f(s/a)=6\exp(-\pi s^2/2a^2)$, period 20 Å, Mo $K\alpha$ radiation, $h_{max}=51$, atom coordinates $x=0.07$, 0.14, 0.28, 0.36, 0.48, 0.60, 0.72, 0.80, 0.88, 0.95; p in (9) runs from −500 to 500]. It must be noted that if (2) is violated, *i.e.* the electron density has some spreading out of the boundaries of the unit cell, the DHT becomes approximate.

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