

On the Decomposition of Lattice-Periodic Functions

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The problem of decomposing an arbitrary periodic function defined on an n -dimensional cubic lattice into finite linear combinations of certain primitive functions is considered. Generally, a primitive function is one which periodically assumes only the values ± 1 and 0 . Rather simple necessary and sufficient conditions are derived for such a decomposition and when a decomposition is possible, an algorithm is given which accomplishes it. These results have been used in recent generalizations of the Ewald method.

I. INTRODUCTION

In a study of the classical problem of the calculation of the potential due to an ionic crystal lattice, and in particular, generalizations of the Ewald method (Ref. 1) along the lines of Nijboer and Dewette (Refs. 3, 4), W. J. C. Grant (Ref. 2) proposed the following problem: Suppose we say that an ionic crystal lattice is primitive if for a suitable choice of origin there exist three vectors $\bar{x}_1, \bar{x}_2, \bar{x}_3$ such that the charge at the point $n_1\bar{x}_1 + n_2\bar{x}_2 + n_3\bar{x}_3$ is just $q_0(-1)^{n_1+n_2+n_3}$ for some fixed q_0 and for all triples of integers (n_1, n_2, n_3) and that the charge at all other points is zero. (For example, the ordinary NaCl lattice is primitive with the \bar{x}_i taken to be the unit coordinate vectors and $q_0 = 1$.) The question is then: Which crystal lattices can be decomposed into finite sums of primitive lattices? Different primitive lattices in the decomposition may have different origins and by the sum of two lattices we mean, of course, the component-wise sum.

The object of this paper is threefold:

- (i) The problem is extended to its natural n -dimensional analogue.
- (ii) Rather simple necessary and sufficient conditions are given for the existence of the desired decomposition.

(iii) When such a decomposition is possible, an algorithm is given which accomplishes it.

II. PRELIMINARY IDEAS

In order to illustrate the basic ideas which will be used in the proofs of the general (n -dimensional) theorem (see p. 1200), we begin by considering the following one-dimensional version.

Suppose we call a real-valued function f defined on the integers *primitive* if for some integers x and c it is true that

$$f(z) = \begin{cases} (-1)^a & \text{if } z = ax + c \\ 0 & \text{otherwise} \end{cases}$$

for all integers a . The question then becomes: What is the set of all those functions which can be represented as real finite linear combinations* of primitive functions? For example, the function g defined by:

$$g(z) = \begin{cases} 0 & \text{if } z \equiv 0 \pmod{4} \\ 1 & \text{if } z \equiv 1 \pmod{4} \\ 2 & \text{if } z \equiv 2 \pmod{4} \\ -3 & \text{if } z \equiv 3 \pmod{4} \end{cases}$$

may be decomposed into a linear combination of primitive functions by:

$$g(z) = -g_1(z) + 2g_2(z) + g_3(z)$$

where

$$g_1(z) = \begin{cases} (-1)^a & \text{if } z = 2a \\ 0 & \text{otherwise} \end{cases},$$

$$g_2(z) = \begin{cases} (-1)^a & \text{if } z = 2a + 1 \\ 0 & \text{otherwise} \end{cases},$$

$$g_3(z) = (-1)^z.$$

We can write this more graphically if we use the notation

$$f: \cdots, a_0, a_1, a_2, \cdots$$

to denote the fact that $f(0) = a_0, f(1) = a_1$, etc. We then have

* In this paper, linear combination will always mean *finite* linear combination.

$$\begin{array}{r}
 -g_1 : \dots, -1, 0, 1, 0, \dots \\
 2g_2 : \dots, 0, 2, 0, -2, \dots \\
 g_3 : \dots, 1, -1, 1, -1, \dots \\
 \hline
 g : \dots, 0, 1, 2, -3, \dots
 \end{array}$$

Similarly, if we start with

$$h : \dots, 1, 3, -2, -1, -3, 2, \dots$$

then the desired decomposition is easily found to be:

$$\begin{array}{r}
 h : \dots, 1, 0, 0, -1, 0, 0, \dots \\
 3h_2 : \dots, 0, 3, 0, 0, -3, 0, \dots \\
 -2h_3 : \dots, 0, 0, -2, 0, 0, 2, \dots \\
 \hline
 h_1 : \dots, 1, 3, -2, -1, -3, 2, \dots
 \end{array}$$

In general, it is clear that any linear combination f of primitive functions is *periodic* and that *within a period the sum of the function values of f must be zero*. If a function has these latter two properties, we say that the function has *mean zero*. It might at first be surmised that any function with mean zero could be written as a linear combination of primitive functions. However, attempts to decompose the periodic function

$$g : \dots, \overline{1, -1, 0, 1, -1, 0}, \dots$$

(the bar indicating a complete period) soon lead one to suspect that this initial guess is incorrect. (In fact, g cannot be decomposed into primitive functions.)

One question which arises immediately is exactly which periods the primitive components of a function f might have, if f itself has some period p (where we say that f has period p if $f(z + p) = f(z)$ for all z). In the preceding example, while g has period 3, perhaps there is a decomposition of g for which the primitive components have much larger periods. (It will turn out, however, that this is not possible.)

To answer these questions, we first introduce some notation. If g is a function defined on the integers,* then by $g(z/r)$ we mean the function defined by:

$$g\left(\frac{z}{r}\right) = \begin{cases} g\left(\frac{z}{r}\right) & \text{if } \frac{z}{r} \text{ is an integer} \\ 0 & \text{otherwise} \end{cases}$$

* In general, in this paper all functions assume the value 0 on points with non-integral coordinates.

Let $i(z)$ denote the function which assumes the value 1 on all integers. Thus, if the function f which we wish to decompose has period

$$p = 2^a(2m + 1),$$

then by forming the functions $i[(z - k)/(2m + 1)]f(z)$, $0 \leq k < 2m + 1$, we have functions which "sample" f at points separated by a distance of $2m + 1$. For example, if f is given by

$$f: \dots, \overline{1, 3, -6, 3, -5, 4, 1, 3, -6, 3, -5, 4, \dots}$$

so that the period of f is $6 = 2 \cdot 3$ (where we will assume that $f(0) = 1$) then we have

$$\begin{aligned} i\left(\frac{z}{3}\right)f(z) &: \dots, \overline{1, 0, 0, 3, 0, 0, \dots} \\ i\left(\frac{z-1}{3}\right)f(z) &: \dots, \overline{0, 3, 0, 0, -5, 0, \dots} \\ i\left(\frac{z-2}{3}\right)f(z) &: \dots, \overline{0, 0, -6, 0, 0, 4, \dots} \end{aligned}$$

Note that $i[(z - k)/(2m + 1)]f(z)$ also has period p and, in general,

$$f(z) = \sum_{k=0}^{2m} i\left(\frac{z - k}{2m + 1}\right)f(z).$$

The result toward which the remainder of this section will be devoted can now be expressed simply in the following way: If f has period

$$p = 2^a(2m + 1)$$

then f can be expressed as a linear combination of primitive functions if and only if for each k the function $i[(z - k)/(2m + 1)]f(z)$ has mean zero.

It follows from this, for example, that if $p = 2^a$ then f can be decomposed into primitive functions if f has mean zero. On the other hand, if f has an odd period $p = 2m + 1$, then each function $i[(z - k)/(2m + 1)]$ has just one nonzero value per period so that f can be decomposed into primitive function if it is identically zero.

We now give a series of lemmas, informal proofs and examples which will indicate the ideas needed for the proof of the general theorem. An outline of our plan of attack is to establish the following results:

If f is a linear combination of primitive functions then for any k and for any $r \neq 0$, $f[(z - k)/r]$ also is a linear combination of primitive functions.

(1)

If f is a linear combination of primitive functions and f has period $p = 2^a(2m + 1)$ then for all k , $i[(z - k)/(2m + 1)]f(z)$ (2) has mean zero.

If f has period 2^a and mean zero then f is a linear combination (3) of primitive functions.

Assuming we have established (1), (2) and (3), the proof of the original assertion follows directly. One direction follows immediately from (2). To show the other direction assume that for each k , $i[(z - k)/(2m + 1)]f(z)$ has mean zero. Notice that each function $i[(z - k)/(2m + 1)]f(z)$ is just an "expanded" copy of a function $f_k(z)$ which has period 2^a and mean zero (i.e., $i[(z - k)/(2m + 1)]f(z) = f_k[(z - k)/(2m + 1)]$). Hence, by (3), $f_k(z)$ is a linear combination of primitive functions and it then follows by (1) that this is also true of $f_k[(z - k)/(2m + 1)]$. Consequently

$$f(z) = \sum_{k=0}^{2m} i \left(\frac{z - k}{2m + 1} \right) f(z) = \sum_{k=0}^{2m} f_k \left(\frac{z - k}{2m + 1} \right)$$

is a linear combination of primitive functions and the proof is completed.

It remains to prove (1), (2) and (3).

The proof of (1) is straightforward. We first note that if $f(z)$ is primitive then $f[(z - k)/r]$ is also primitive for any k and for any $r \neq 0$. For by hypothesis there exist x and c such that

$$f(z) = \begin{cases} (-1)^a & \text{if } z = ax + c \\ 0 & \text{otherwise} \end{cases}$$

On the other hand, by definition we have

$$f \left(\frac{z - k}{r} \right) = \begin{cases} f(y) & \text{if } z = ry + k \\ 0 & \text{otherwise} \end{cases}$$

Hence

$$\begin{aligned} f \left(\frac{z - k}{r} \right) &= \begin{cases} (-1)^a & \text{if } z = r(ax + c) + k \\ 0 & \text{otherwise} \end{cases} \\ &= \begin{cases} (-1)^a & \text{if } z = a(rx) + (rc + k) \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

and so $f[(z - k)/r]$ is primitive. The extension to linear combinations of primitive functions follows at once and (1) is proved.

In order to prove (2) we first need an auxiliary result (a simplified version of Lemma 2). This is: Suppose f has periods $p = 2^a(2m + 1)$

and $p' = 2^a(2m' + 1)$. Then for any k , $i[(z - k)/(2m + 1)]f(z)$ has mean zero iff $i[(z - k)/(2m' + 1)]f(z)$ has mean zero. To prove this, let us first assume that $a' = a$ and $2m + 1$ divides $2m' + 1$. The sum $\sum_{z=0}^{p-1} i[(z - k)/(2m + 1)]f(z)$ is exactly the sum of the $f(z)$ for which $z - k \equiv 0 \pmod{2m + 1}$, and $0 \leq z - k \leq p - 1$ (since $i[(z - k)/(2m + 1)]f(z)$ has period p). There are 2^a such values of $z - k$, namely,

$$z - k \in A = \{0, 2m + 1, 2(2m + 1), \dots, (2^a - 1)(2m + 1)\}.$$

Similarly the sum $\sum_{z=0}^{p'-1} i[(z - k)/(2m' + 1)]f(z)$ is exactly the sum of the $f(z)$ for which $z - k \equiv 0 \pmod{2m' + 1}$ and $0 \leq z - k \leq p' - 1$. Again there are 2^a such values of $z - k$, namely,

$$z - k \in B = \{0, 2m' + 1, 2(2m' + 1), \dots, (2^a - 1)(2m' + 1)\}.$$

All the elements of A and B are congruent to zero modulo $2m + 1$ (since $2m + 1$ divides $2m' + 1$). Also since $2m + 1$ and $2m' + 1$ are odd then both sets A and B contain a complete residue system modulo 2^a . Hence modulo p , A and B are identical. Since f has period p then

$$\sum_{z=0}^{p-1} i\left(\frac{z - k}{2m + 1}\right)f(z) = \sum_{z \in A} f(z) = \sum_{z \in B} f(z) = \sum_{z=0}^{p'-1} i\left(\frac{z - k}{2m' + 1}\right)f(z).$$

If we now assume that $a' \geq a$ (instead of $a' = a$) then it is not difficult to see that

$$\sum_{z=0}^{p'-1} i\left(\frac{z - k}{2m' + 1}\right)f(z) = 2^{a'-a} \sum_{z=0}^{p-1} i\left(\frac{z - k}{2m + 1}\right)f(z).$$

Thus, what we have shown is that if f has periods $p = 2^a(2m + 1)$ and $p' = 2^{a'}(2m' + 1)$ where p divides p' then $i[(z - k)/(2m + 1)]f(z)$ has mean zero iff $i[(z - k)/(2m' + 1)]f(z)$ has mean zero. Since in general a function which has periods q and q' also has period (q, q') (the greatest common divisor of q and q'), then the initial assertion follows at once. As a simple example consider the function f given by

$$f: \dots, \overline{1, 3, -2, -1, 4, 2, 1, 3, -2, -1, 4, 2}, \dots.$$

This function has $6 = 2 \cdot 3$ as a period and $i(z/3)f(z)$ has mean zero since

$$\sum_{z=0}^5 i(z/3)f(z) = f(0) + f(3) = 1 - 1 = 0.$$

However we may also consider f as having a period of $12 = 2^2 \cdot 3$ in which case $i(z/3)f(z)$ has also mean zero since

$$\sum_{z=0}^{11} i(z/3)f(z) = f(0) + f(3) + f(6) + f(9) = 0.$$

Finally, f has a period of $18 = 2 \cdot 3^2$ and $i(z/9)f(z)$ still has mean zero since

$$\sum_{z=0}^{17} i(z/9)f(z) = f(0) + f(9) = 0.$$

Our next step will be to prove (2) using the result just established. We first show that if f is *primitive* and has period $p = 2^a(2m + 1)$ then

$$\sum_{z=0}^{p-1} i\left(\frac{z-k}{2m+1}\right)f(z) = 0 \quad \text{for all } k. \quad (4)$$

To see this, we partition the integers into two-element subsets $\{u_i, v_i\}$ such that $v_i = u_i + 2m + 1$ for each i . Since f is primitive there exist integers x and c such that

$$f(z) = \begin{cases} (-1)^a & \text{if } z = ax + c \\ 0 & \text{otherwise} \end{cases}.$$

Since

$$u_i x \equiv v_i x \pmod{2m+1}$$

and $v_i - u_i = 2m + 1$ is odd then it follows that

$$f(u_i x + c) = -f(v_i x + c) \quad \text{for all } i.$$

But

$$i\left(\frac{u_i x - k}{2m+1}\right) = i\left(\frac{v_i x - k}{2m+1}\right) \quad \text{for all } i \text{ and } k.$$

Consequently it follows from the fact that f has period p that

$$\sum_{z=0}^{p-1} i\left(\frac{z-k}{2m+1}\right)f(z) = 0 \quad \text{for all } k$$

and (4) is established.

To establish (2) assume that f has period $p = 2^a(2m + 1)$ and is a linear combination of primitive functions f_i , $1 \leq i \leq t$. If f_i has period $p_i = 2^{a_i}(2m_i + 1)$ then by (4) we know that

$$\sum_{z=0}^{p_i-1} i\left(\frac{z-k}{2m_i+1}\right)f_i(z) = 0 \quad \text{for all } k.$$

Hence, if we choose $q = p_1 p_2 \cdots p_t p = 2^{a'} (2m' + 1)$ then by the simplified version of Lemma 2, we have

$$\sum_{z=0}^{q-1} i \left(\frac{z - k}{2m' + 1} \right) f_i(z) = 0 \quad \text{for } 1 \leq i \leq t \quad \text{and all } k.$$

Consequently

$$\sum_{z=0}^{q-1} i \left(\frac{z - k}{2m' + 1} \right) f(z) = 0$$

since by hypothesis f is a linear combination of the f_i . But f has period p so applying the Lemma 2 result again we find

$$\sum_{z=0}^{p-1} i \left(\frac{z - k}{2m + 1} \right) f(z) = 0$$

and (2) is proved.

We are left with (3) to prove. To do this we first establish the following result: If $h(z)$ is defined by $h(z) = (-1)^z$ then for a fixed n , the $2^n - 1$ functions $h[(z - k)/2^r]$, $0 \leq k < 2^r$, $0 \leq r < n$, are linearly independent over the reals. This is easy to see since for a fixed r , $h[(z - k)/2^r]$ assigns a nonzero value only to those z such that $z \equiv k \pmod{2^r}$. Hence for $k = 0, 1, \dots, 2^r - 1$, the $h[(z - k)/2^r]$ assume nonzero values on disjoint sets. On the other hand, $h[(z - k)/2^r]$ assigns *different* values to the points k and $k + 2^r$ while any $h[(z - k')/2^{r'}]$ assigns the *same* value to these points for $r' < r$. Thus, $h[(z - k)/2^r]$ is not a linear combination of other $h[(z - k)/2^s]$ for $s \leq r$. This establishes the independence of the h 's. Note that for $0 \leq k < 2^r$ and $0 \leq r < n$, the function $h[(z - k)/2^r]$ has period 2^n and mean zero. By taking suitable linear combinations of the $2^n - 1$ independent $h[(z - k)/2^r]$, we can form functions f which assume any desired values on the points $0, 1, 2, \dots, 2^n - 2$. Of course, we must have

$$f(2^n - 1) = - \sum_{z=0}^{2^n-2} f(z).$$

Consequently the $2^n - 1$ functions $h[(z - k)/2^r]$ form a *basis* for the set of all periodic functions with period 2^n and mean zero. That is, any function f with period 2^n and mean zero can be written as a linear combination of primitive functions with period 2^n . This completes the proof of (3).

To conclude this section we give an example which illustrates the ease with which the primitive components of a function may be found. Consider the function g given by:

$$g: \dots, \overline{1, 2, -5, \pi, \frac{1}{2}, 1 - \pi, \frac{1}{2}, 0}, \dots$$

g has period 8 and mean zero. The only component $h[(z - k)/2]$ which can cause a difference in $g(0)$ and $g(4)$ is

$$h(z/4): \dots, 1, 0, 0, 0, -1, 0, 0, 0, \dots$$

Since $\alpha h(z/4)$ assigns the points 0 and 4 values which differ by 2α and

$$g(0) - g(4) = \frac{1}{2}$$

then by choosing $\alpha = \frac{1}{4}$ we obtain the $h(z/4)$ component of g . Performing similar calculations for $h[(z - k)/4]$, $k = 1, 2, 3$, we obtain

$$g_1(z) = g(z) - \frac{1}{4} h\left(\frac{z}{4}\right) - \left(\frac{\pi + 1}{2}\right) h\left(\frac{z - 1}{4}\right) + \frac{11}{4} h\left(\frac{z - 2}{4}\right) - \frac{\pi}{2} h\left(\frac{z - 3}{4}\right)$$

given by

$$g_1(z): \dots, \overline{\frac{3}{4}, \frac{3 - \pi}{2}, -\frac{9}{4}, \frac{\pi}{2}, \frac{3}{4}, \frac{3 - \pi}{2}, -\frac{9}{4}, \frac{\pi}{2}}, \dots$$

(which has period 4). We apply the same arguments to the decomposition of $g_1(z)$ into the $h[(z - k)/2]$, $k = 0, 1$, and find

$$g_2(z) = g_1(z) - \frac{3}{2} h\left(\frac{z}{2}\right) - \left(\frac{3}{4} - \frac{\pi}{2}\right) h\left(\frac{z - 1}{2}\right)$$

given by

$$g_2(z): \dots, \overline{-\frac{3}{4}, \frac{3}{4}, -\frac{3}{4}, \frac{3}{4}, -\frac{3}{4}, \frac{3}{4}, -\frac{3}{4}, \frac{3}{4}}, \dots$$

so that $g_2(z) = -\frac{3}{4}h(z)$. Consequently g has been decomposed into primitive functions. Graphically we have:

$$\begin{array}{cccccccc}
 \frac{1}{4} h\left(\frac{z}{4}\right) : \dots, & \frac{1}{4}, & 0, & 0, & 0, & -\frac{1}{4}, & 0, & 0, & 0, \dots \\
 \left(\frac{\pi+1}{2}\right) h\left(\frac{z-1}{4}\right) : \dots, & 0, & \frac{\pi+1}{2}, & 0, & 0, & 0, & -\left(\frac{\pi+1}{2}\right), & 0, & 0, \dots \\
 -\frac{11}{4} h\left(\frac{z-2}{4}\right) : \dots, & 0, & 0, & -\frac{11}{4}, & 0, & 0, & 0, & \frac{11}{4}, & 0, \dots \\
 \frac{\pi}{2} h\left(\frac{z-3}{4}\right) : \dots, & 0, & 0, & 0, & \frac{\pi}{2}, & 0, & 0, & 0, & -\frac{\pi}{2}, \dots \\
 \frac{3}{2} h\left(\frac{z}{2}\right) : \dots, & \frac{3}{2}, & 0, & -\frac{3}{2}, & 0, & \frac{3}{2}, & 0, & -\frac{3}{2}, & 0, \dots \\
 \left(\frac{3}{4} - \frac{\pi}{2}\right) h\left(\frac{z-1}{2}\right) : \dots, & 0, & \frac{3}{4} - \frac{\pi}{2}, & 0, & \frac{\pi}{2} - \frac{3}{4}, & 0, & \frac{3}{4} - \frac{\pi}{2}, & 0, & \frac{\pi}{2} - \frac{3}{4}, \dots \\
 -\frac{3}{4} h(z) : \dots, & -\frac{3}{4}, & \frac{3}{4}, & -\frac{3}{4}, & \frac{3}{4}, & -\frac{3}{4}, & \frac{3}{4}, & -\frac{3}{4}, & \frac{3}{4}, \dots
 \end{array}$$

$$g(z) : \dots, \quad 1, \quad 2, \quad -5, \quad \pi, \quad \frac{1}{2}, \quad 1 - \pi, \quad \frac{1}{2}, \quad 0, \dots$$

III. THE GENERAL THEOREM

We are ready to proceed to the n -dimensional generalizations of the results of Section II. The proofs given will use basically the same ideas as before although the technical details become somewhat more formal and involved. We begin with some definitions.

Let Z^n denote the ring of n -tuples of integers with component-wise addition and multiplication. That is, if $a = (a_1, \dots, a_n)$ and $b = (b_1, \dots, b_n)$ are elements of Z^n then

$$a + b = (a_1 + b_1, \dots, a_n + b_n)$$

and

$$a \cdot b = (a_1 \cdot b_1, \dots, a_n \cdot b_n).$$

In general, unless otherwise noted, lower case Latin letters without subscripts will denote elements of Z^n ; lower case letters with subscripts will denote elements of Z , i.e., integers. If $\alpha \in Z$ and $q = (q_1, q_2, \dots, q_n) \in Z^n$ then we define αq to be $(\alpha q_1, \alpha q_2, \dots, \alpha q_n)$. The n -tuple $(1, 1, \dots, 1)$ will be denoted by e . By $a < b$ we mean $a_i < b_i$ for $1 \leq i \leq n$.

A function $f: Z^n \rightarrow R$ (the real numbers) is said to be *primitive* if there exist $a, x^{(1)}, \dots, x^{(n)} \in Z^n$ such that

$$f(z) = \begin{cases} (-1)^{c_1+\dots+c_n} & \text{if } z = c_1x^{(1)} + \dots + c_nx^{(n)} + a \\ 0 & \text{otherwise} \end{cases}$$

for all $z \in Z^n$.

Let \mathcal{G} denote the real vector space generated by the set of all primitive functions. Z^{n+} will denote the subset of Z^n consisting of those n -tuples which have all *positive* coordinates. If $m \in Z^{n+}$ then P_m is defined by

$$P_m = \{x \in Z^n: 0 \leq x < m\}$$

(i.e., $0 \leq x_i < m_i$ for $1 \leq i \leq n$, where 0 will be used to designate both an element of Z and also the n -tuple $(0, 0; \dots, 0)$.)

A function $f: Z^n \rightarrow R$ is said to have *period* m if

$$f(z + km) = f(z) \quad \text{for all } z, k \in Z^n.$$

If f has period m and

$$\sum_{z \in P_m} f(z) = 0$$

then f is said to have *mean zero*. Let \mathfrak{F}_m denote the real vector space of all functions of period m which have mean zero. Next, we define

$$f[(z - a)/b], \quad b \neq 0,$$

by

$$f\left(\frac{z - a}{b}\right) = \begin{cases} f(y) & \text{if } z = by + a \\ 0 & \text{otherwise} \end{cases}.$$

For $\alpha \in Z, \alpha \neq 0$, let $E(\alpha)$ and $O(\alpha)$ denote the “even part” and “odd part” of α respectively. In other words, if $\alpha = 2^\beta(2\mu + 1)$ for $\beta, \mu \in Z$ then $E(\alpha) = 2^\beta$ and $O(\alpha) = 2\mu + 1$. For $m = (m_1, \dots, m_n) \in Z^n$, $E(m)$ will denote the n -tuple $(E(m_1), \dots, E(m_n))$ with $O(m)$ defined similarly.

Finally, for $m \in Z^n$, let \mathfrak{F}_m^* denote the real vector space generated by the set of functions

$$\left\{ f\left(\frac{z - a}{O(m)}\right) : f \in \mathfrak{F}_{E(m)}, a \in Z^n \right\}.$$

We note that if $m = e = (1, 1, \dots, 1)$ then $\mathfrak{F}_m^* = \mathfrak{F}_m$; in general, we always have $\mathfrak{F}_m^* \subset \mathfrak{F}_m$.

We come now to the main result of the paper. This is the following:

Theorem.

$$\mathfrak{G} \cap \mathfrak{F}_m = \mathfrak{F}_m^*$$

for $m \in Z^{n+}$.

The proof of this theorem will proceed in a series of Lemmas paralleling the steps taken in the preceding section.

Lemma 1. If $g(z) \in \mathfrak{G}$ then $g[(z - a)/r] \in \mathfrak{G}$ for all $a \in Z^n$ and $r \in Z^{n+}$.

Proof. We first show that if $f(z)$ is primitive then $f[(z - a)/r]$ is primitive. If we assume $f(z)$ is primitive then by definition there exist $b, x^{(1)}, \dots, x^{(n)} \in Z^n$ such that

$$f(z) = \begin{cases} (-1)^{c_1 + \dots + c_n} & \text{if } z = c_1 x^{(1)} + \dots + c_n x^{(n)} + b. \\ 0 & \text{otherwise} \end{cases}$$

On the other hand

$$f\left(\frac{z - a}{r}\right) = \begin{cases} f(y) & \text{if } z = ry + a \\ 0 & \text{otherwise} \end{cases}.$$

Therefore

$$\begin{aligned} f\left(\frac{z - a}{r}\right) &= \begin{cases} (-1)^{c_1 + \dots + c_n} & \text{if } z = r(c_1 x^{(1)} + \dots + c_n x^{(n)} + b) + a \\ 0 & \text{otherwise} \end{cases} \\ &= \begin{cases} (-1)^{c_1 + \dots + c_n} & \text{if } z = c_1(rx^{(1)}) + \dots + c_n(rx^{(n)}) + rb + a \\ 0 & \text{otherwise} \end{cases} \end{aligned}$$

and hence, $f[(z - a)/r]$ is primitive. By applying this result to a linear combination of primitive functions, i.e., an element of \mathfrak{G} , the lemma follows.

Let $i, \pi: Z^n \rightarrow R$ be defined by

$$i(z) = 1, \quad \pi(z) = z_1 z_2 \dots z_n \quad \text{for all } z = (z_1, z_2, \dots, z_n) \in Z^n.$$

Lemma 2. Let $c, m \in Z^{n+}$, $r = cm$ and suppose $f: Z^n \rightarrow R$ has period m . Then for any $a \in Z^n$

$$\sum_{z \in P_r} i \left(\frac{z - a}{O(r)} \right) f(z) = \pi(E(c)) \sum_{z \in P_m} i \left(\frac{z - a}{O(m)} \right) f(z).$$

Proof. We first note that since

$$\begin{aligned} r &= cm = E(c)O(c)E(m)O(m) \\ &= E(c)E(m)O(c)O(m) = E(r)O(r) \end{aligned}$$

then

$$E(r) = E(c)E(m) \quad \text{and} \quad O(r) = O(c)O(m).$$

By definition

$$\sum_{z \in P_{O(c)m}} i \left(\frac{z - a}{O(O(c)m)} \right) f(z) = \sum_{z \in A} f(z)$$

and

$$\sum_{z \in P_m} i \left(\frac{z - a}{O(m)} \right) f(z) = \sum_{z \in B} f(z)$$

where

$$A = \{z: 0 \leq z = kO(c)O(m) + a < O(c)m \quad \text{for some } k\}$$

and

$$B = \{z: 0 \leq z = kO(m) + a < m \quad \text{for some } k\}.$$

Hence, for each set, the values which k may assume are just a translation of $P_{E(m)}$, there being $\pi(E(m))$ values in all. Since $O(m)$ and $O(c)O(m)$ are odd (i.e., each component is odd), then A and B both contain a *complete residue system modulo* $E(m)$. Consequently, since all the elements of A and B are congruent to a modulo $O(m)$ then *modulo* $E(m)O(m)$, A and B are identical. Since $m = E(m)O(m)$ and f has period m then the sums $\sum_{z \in A} f(z)$ and $\sum_{z \in B} f(z)$ are equal.

We also note in general that for any $s \in \mathbb{Z}^{n+}$

$$\sum_{P_{E(c)s}} i \left(\frac{z - a}{O(s)} \right) f(z) = \pi(E(c)) \sum_{P_s} i \left(\frac{z - a}{O(s)} \right) f(z)$$

since $P_{E(c)s}$ is the disjoint union of $\pi(E(c))$ copies of P_s . Therefore we have

$$\begin{aligned} \sum_{P_r} i \left(\frac{z-a}{O(r)} \right) f(z) &= \sum_{P_{cm}} i \left(\frac{z-a}{O(cm)} \right) f(z) \\ &= \sum_{P_{E(c)O(c)m}} i \left(\frac{z-a}{O(c)O(m)} \right) f(z) \\ &= \pi(E(c)) \sum_{P_{O(c)m}} i \left(\frac{z-a}{O(c)O(m)} \right) f(z) \\ &= \pi(E(c)) \sum_{P_m} i \left(\frac{z-a}{O(m)} \right) f(z) \end{aligned}$$

and the lemma is proved.

We should note that as a corollary to this lemma we obtain:

$$i \left(\frac{z-a}{cm} \right) f(z) \text{ has mean zero iff} \tag{5}$$

$$i \left(\frac{z-a}{m} \right) f(z) \text{ has mean zero.}$$

We are now in a position to prove the important

Lemma 3. Suppose $g \in \mathfrak{G}$ has period $p \in Z^{n+}$. Then for all $a \in Z^n$,

$$\sum_{P_p} i \left(\frac{z-a}{O(p)} \right) g(z) = 0.$$

Proof. We first show that the above conclusion holds if we assume that $g = f$ is primitive with period $q = (\alpha, \alpha, \dots, \alpha)$. In this case there exists $c, x^{(1)}, \dots, x^{(n)} \in Z^n$ such that

$$f(z) = \begin{cases} (-1)^{a_1 + \dots + a_n} & \text{if } z = a_1 x^{(1)} + \dots + a_n x^{(n)} + c \\ 0 & \text{otherwise} \end{cases}$$

To each $u = (u_1, \dots, u_n) \in Z^n$ we can associate the *unique* point $v = (v_1, \dots, v_n) \in Z^n$ such that $v_1 = u_1 \pm O(q)$, $v_i = u_i$ for $i > 1$, where the \pm sign is chosen so that Z^n is decomposed into the union of disjoint pairs $\{u, v\}$. It follows at once that

$$u_1 x^{(1)} + \dots + u_n x^{(n)} \equiv v_1 x^{(1)} + \dots + v_n x^{(n)} \pmod{O(q)}.$$

Since

$$\sum_{i=1}^n v_i - \sum_{i=1}^n u_i = \pm O(q)$$

is odd then

$$f(u_1x^{(1)} + \dots + u_nx^{(n)} + c) = -f(v_1x^{(1)} + \dots + v_nx^{(n)} + c).$$

Also, note that for all $a \in Z^n$

$$i\left(\frac{u_1x^{(1)} + \dots + u_nx^{(n)} - a}{O(q)}\right) = i\left(\frac{v_1x^{(1)} + \dots + v_nx^{(n)} - a}{O(q)}\right).$$

Since f has period q then we must have

$$\sum_{P_q} i\left(\frac{z - a}{O(q)}\right) f(z) = 0$$

as asserted.

We may now remove the restriction that f has period of the form $q = (\alpha, \alpha, \dots, \alpha) = \alpha e$. If we assume f has an arbitrary period $p \in Z^{n+}$ then it is certainly true that f also has period $\pi(p)e$. By above we have

$$\sum_{P_{\pi(p)e}} i\left(\frac{z - a}{O(\pi(p)e)}\right) f(z) = 0.$$

Since p divides $\pi(p)e$ then by (5) we see that

$$\sum_{P_p} i\left(\frac{z - a}{O(p)}\right) f(z) = 0. \tag{6}$$

Finally, to prove the lemma assume that

$$g = \sum_{j=1}^t \alpha_j f_j$$

where the α_j are real and the f_j are primitive. If f_j has period $p^{(j)}$ then by (6) we have

$$\sum_{P_{p^{(j)}}} i\left(\frac{z - a}{O(p^{(j)})}\right) f_j(z) = 0 \quad \text{for } 1 \leq j \leq t.$$

If g has period p and q denotes $p^{(1)}p^{(2)} \dots p^{(t)}p$ then by Lemma 2

$$\sum_{P_q} i\left(\frac{z - a}{O(q)}\right) f_j(z) = 0 \quad \text{for } 1 \leq j \leq t.$$

Therefore

$$\sum_{P_q} i\left(\frac{z - a}{O(q)}\right) g(z) = \sum_{j=1}^t \alpha_j \sum_{P_q} i\left(\frac{z - a}{O(q)}\right) f_j(z) = 0$$

so that applying Lemma 2 again we obtain

$$\sum_{P_p} i\left(\frac{z - a}{O(p)}\right) g(z) = 0$$

since g has period p . This proves the lemma.

The final lemma is an n -dimensional generalization of (3). Its proof, however, is considerably more complicated.

Lemma 4. If $m = 2^\alpha e$ for some $\alpha \in Z^+$ then $\mathfrak{F}_m \subset \mathfrak{G}$.

Proof. It will be sufficient to show that there exist $2^{n\alpha} - 1$ functions in \mathfrak{G} which also belong to \mathfrak{F}_m and which are linearly independent over R . Let $C^{(k)}$ denote the $k \times k$ matrix of the form

$$C^{(k)} = \begin{pmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 1 & -1 & 1 & 1 & \cdots & 1 \\ 1 & 1 & -1 & 1 & \cdots & 1 \\ 1 & 1 & 1 & -1 & \cdots & 1 \\ \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\ 1 & 1 & 1 & 1 & \cdots & -1 \end{pmatrix}$$

and let $D^{(k)}$ denote the $k \times k$ matrix of the form

$$D^{(k)} = \begin{pmatrix} 0 & 0 & 0 & \cdots & 0 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 1 \\ 0 & 0 & 0 & \cdots & 1 & 1 & 1 \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot & \cdot & \cdot \\ 1 & 1 & 1 & \cdots & 1 & 1 & 1 \end{pmatrix}$$

In other words,

$$c_{ij} = \begin{cases} 1 & \text{for } i = 1 \\ 1 - 2\delta_{ij} & \text{for } i > 1 \end{cases}$$

and

$$d_{ij} = \begin{cases} 0 & \text{if } i + j \leq k \\ 1 & \text{otherwise} \end{cases}$$

where δ_{ij} is the Kronecker δ -function. Define $B_\kappa^{(\nu)}$ to be the $\nu \times \nu$ matrix of the form

$$B_\kappa^{(\nu)} = \begin{pmatrix} \mathbf{0} & C^{(\nu-\kappa+1)} \\ D^{(\kappa-1)} & \mathbf{0} \end{pmatrix} \text{ for } 1 \leq \kappa \leq \nu$$

where $\mathbf{0}$ denotes the appropriate zero matrix. Let $r_{\kappa,\lambda}^{(\nu)}$ denote the point of Z^ν formed from the λ th row of $B_\kappa^{(\nu)}$. Finally, let $f_\kappa^{(\nu)}$ denote the function in \mathcal{G} defined by

$$f_\kappa^{(\nu)}(z) = \begin{cases} (-1)^{a_1+\dots+a_n} & \text{if } z = a_1 r_{\kappa,1}^{(\nu)} + \dots + a_n r_{\kappa,\nu}^{(\nu)} \\ \mathbf{0} & \text{otherwise} \end{cases}$$

We show first that the functions $f_\kappa^{(\nu)}$, $1 \leq \kappa \leq \nu$, are linearly independent over R . To accomplish this it suffices to show that for any κ , $1 \leq \kappa \leq \nu$, there are two points p and q in Z^ν such that

$$f_\kappa^{(\nu)}(p) \neq f_\kappa^{(\nu)}(q)$$

while

$$f_\tau^{(\nu)}(p) = f_\tau^{(\nu)}(q) \text{ for } \kappa < \tau \leq \nu.$$

What we show in fact is that if $|f_\kappa^{(\nu)}(p)| = 1$ then $f_{\kappa+1}^{(\nu)}(p) = 1$ for $1 \leq \kappa < \nu$. This may be proved by showing that if $s \in Z^\nu$ is any Z -linear combination of the $r_{\kappa,\lambda}^{(\nu)}$, $1 \leq \lambda \leq \nu$, then s can be written as a Z -linear combination of the $r_{\kappa+1,\lambda}^{(\nu)}$, $1 \leq \lambda \leq \nu$, such that the sum of the coefficients is divisible by 2. We proceed by induction on ν . For $\nu = 2$ we have

$$B_1^{(2)} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad B_2^{(2)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Since

$$r_{1,1}^{(2)} = r_{2,1}^{(2)} + r_{2,2}^{(2)}$$

and

$$r_{1,2}^{(2)} = r_{2,2}^{(2)} - r_{2,1}^{(2)}$$

then any Z -linear combination of the $r_{1,\lambda}^{(2)}$ can be written as a Z -linear combination of the $r_{2,\lambda}^{(2)}$ with the sum of the coefficients divisible by 2 and the assertion is true for this case. Now assume the hypothesis for ν and let

$$\begin{aligned}
 s &= \sum_{\lambda=1}^{\nu} a_{\lambda} r_{1,\lambda}^{(\nu+1)} + a_{\nu+1} r_{1,\nu+1}^{(\nu+1)} \\
 &= \sum_{\lambda=1}^{\nu} b_{\lambda} r_{2,\lambda}^{(\nu+1)} + a_{\nu+1} (r_{2,\nu}^{(\nu+1)} + r_{2,\nu+1}^{(\nu+1)})
 \end{aligned}$$

which expresses s as a Z -linear combination of the $r_{2,\lambda}^{(\nu+1)}$ with an even coefficient sum. This completes the induction step and the proof of the assertion that the $f_{\kappa}^{(\nu)}$, $1 \leq \kappa \leq \nu$, are linearly independent over R .

A more careful examination of $B_{\kappa}^{(\nu)}$ reveals the following:

- (a) $r_{\kappa,\lambda+1}^{(\nu)} - r_{\kappa,\lambda}^{(\nu)} = (\delta_{1,\nu-\lambda}, \delta_{2,\nu-\lambda}, \dots, \delta_{\nu,\nu-\lambda})$
for $\nu - \kappa + 1 \leq \lambda \leq \nu - 1$.
- (b) $r_{\kappa,1}^{(\nu)} - r_{\kappa,\lambda}^{(\nu)} = (2\delta_{1,\kappa+\lambda-1}, 2\delta_{2,\kappa+\lambda-1}, \dots, 2\delta_{\nu,\kappa+\lambda-1})$
for $2 \leq \lambda \leq \nu - \kappa + 1$.
- (c) $\sum_{\lambda=2}^{\nu-\kappa} r_{\kappa,\lambda}^{(\nu)} - (\nu - \kappa - 2)r_{\kappa,1}^{(\nu)} = (2\delta_{1,\kappa}, 2\delta_{2,\kappa}, \dots, 2\delta_{\nu,\kappa})$.

Since the linear combinations of the $r_{\kappa,\lambda}^{(\nu)}$ in (a), (b) and (c) all have the sum of coefficients an even integer then

$$f_{\kappa}^{(\nu)}((2\delta_{1,\lambda}, 2\delta_{2,\lambda}, \dots, 2\delta_{\nu,\lambda})) = f_{\kappa}^{(\nu)}(0)$$

for $1 \leq \lambda, \kappa \leq \nu$. Hence $f_{\kappa}^{(\nu)}$ has period $2e = (2, 2, \dots, 2)$. Also we note that the only points in $P_{2e} \subset Z^{\nu}$ at which $f_{\kappa}^{(\nu)}$ is nonzero are just those Z -linear combinations of the $r_{\kappa,\lambda}^{(\nu)}$ which have all coordinates 0 or 1. It is not difficult to see that the only points of this type which may be generated are the 2^{κ} points of the form $(c_1, c_2, \dots, c_{\kappa-1}, c_0, c_0, \dots, c_0)$ where $c_j = 0$ or 1. By a translation of $f_{\kappa}^{(\nu)}$ by a we mean the function $f_{\kappa,a}^{(\nu)}$ defined by

$$f_{\kappa,a}^{(\nu)}(z) = f_{\kappa}^{(\nu)}(z - a).$$

By letting the a range over the set of points

$$A_{\kappa} = \{(\underbrace{0, 0, \dots, 0}_{\kappa}, d_1, d_2, \dots, d_{\nu-\kappa}) : d_{\lambda} = 0 \text{ or } 1\},$$

the $2^{\nu-\kappa}$ translations $f_{\kappa,a}^{(a)}$, $a \in A_{\kappa}$, have the property that for each $p \in P_{2e}$, exactly one of the $f_{\kappa,a}^{(\nu)}$ assumes a nonzero value at p . In fact, if we define an inner product $(f_{\kappa,a}^{(\nu)}, f_{\lambda,b}^{(\nu)})$ for $f_{\kappa,a}^{(\nu)}$ and $f_{\lambda,b}^{(\nu)}$ by

$$(f_{\kappa,a}^{(\nu)}, f_{\lambda,b}^{(\nu)}) = \sum_{p \in P_{2e}} f_{\kappa,a}^{(\nu)}(p) f_{\lambda,b}^{(\nu)}(p)$$

then the inner product of any two distinct functions $f_{\kappa,a}^{(\nu)}, f_{\lambda,b}^{(\nu)}$, $a \in A_{\kappa}$, $b \in A_{\lambda}$, $1 \leq \kappa, \lambda \leq \nu$, is zero. Since

$$(f_{\kappa,a}^{(\nu)}, f_{\kappa,a}^{(\nu)}) = 2^{\kappa}$$

then by introducing the “normalized” basis functions

$$\hat{f}_{\kappa,a}^{(\nu)} = 2^{-\kappa/2} f_{\kappa,a}^{(\nu)}$$

we see that the set of $(1 + 2 + \dots + 2^{\nu-1}) = 2^\nu - 1$ functions $\hat{f}_{\kappa,a}^{(\nu)}$, $a \in A_\kappa$, $1 \leq \kappa \leq \nu$, are orthonormal. Thus, we have shown that $F_{2^\alpha} \subset \mathfrak{G}$.

The extension of this technique to show that $F_{2^\alpha} \subset \mathfrak{G}$ is quite similar and will be omitted. The basic idea is simply to introduce the “expansions” $f_{\kappa,a,\lambda}^{(\nu)}$ of $f_{\kappa,a}^{(\nu)}$ defined by

$$f_{\kappa,a,\lambda}^{(\nu)}(z) = f_{\kappa,a}^{(\nu)}(z/\lambda) \quad \text{for } \lambda = 2^0, 2^1, \dots, 2^{\alpha-1},$$

and then by taking suitable normalized translations of these functions, obtain an orthonormal basis (in \mathfrak{G}) for \mathfrak{F}_{2^α} . This shows that

$$\mathfrak{F}_m = \mathfrak{F}_{2^\alpha} \subset \mathfrak{G}$$

and the proof of the lemma is completed.

We are now ready to proceed to the proof of the

Theorem.

$$\mathfrak{G} \cap \mathfrak{F}_m = \mathfrak{F}_m^*$$

for $m \in \mathbb{Z}^{n+}$.

Proof: $\mathfrak{G} \cap \mathfrak{F}_m \subset \mathfrak{F}_m^*$

Let $f \in \mathfrak{G} \cap \mathfrak{F}_m$. Since f has period m then by Lemma 3, we have for all $a \in \mathbb{Z}^n$

$$\sum_{z \in \mathfrak{F}_m} i \left(\frac{z - a}{O(m)} \right) f(z) = 0.$$

Since

$$f(z) = \sum_{a \in \mathfrak{F}_{O(m)}} i \left(\frac{z - a}{O(m)} \right) f(z)$$

and each of the functions $i[(z - a)/O(m)]f(z)$ can be written as $h[(z - a)/O(m)]$ for some $h \in \mathfrak{F}_{\mathfrak{B}(m)}$ then $f \in \mathfrak{F}_m^*$ and this direction is established.

$$\mathfrak{G} \cap \mathfrak{F}_m \supset \mathfrak{F}_m^*$$

We have already noted that $\mathfrak{F}_m^* \subset \mathfrak{F}_m$. It remains to show that $\mathfrak{F}_m^* \subset \mathfrak{G}$. By definition \mathfrak{F}_m^* is the real vector space generated by the set

$$\{h[(z - a)/O(m)]: h \in \mathfrak{F}_{\mathfrak{B}(m)}, a \in \mathbb{Z}^n\}.$$

By Lemma 4 we have

$$\mathfrak{F}_{E(m)} \subset \mathfrak{F}_{\pi(E(m))e} \subset \mathfrak{G}.$$

Thus, if $h \in \mathfrak{F}_{E(m)}$ then $h \in \mathfrak{G}$. But by Lemma 1, $h \in \mathfrak{G}$ implies

$$h[(z - a)/O(m)] \in \mathfrak{G}.$$

Therefore, since \mathfrak{G} contains a set of generators for \mathfrak{F}_m^* then $\mathfrak{F}_m^* \subset \mathfrak{G}$. This completes the proof of the theorem.

IV. CONCLUDING REMARKS

As a concluding example of the results of the preceding section, we consider the decomposition of the function f generated by the charge distribution of the crystal structure of potassium tantalate, KTaO_3 . This compound forms face-centered cubic crystals with a charge distribution as shown in Fig. 1. That is, a +1 is situated at each vertex, a -2 at each face-center and a +5 is located in the center of the cube. The periodic function f defined by this distribution has period (2,2,2) and is shown in Fig. 2 (which is the forward upper left octant of Fig. 1). We have

$$B_1^{(3)} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \quad B_2^{(3)} = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 1 & -1 \\ 1 & 0 & 0 \end{pmatrix}, \quad B_3^{(3)} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 1 & 0 \end{pmatrix}$$

so that the 7 basis functions into which f will be decomposed are as shown in Fig. 3.

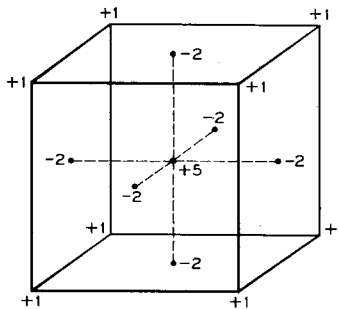


Fig. 1 — Charge distribution of KTaO_3 .

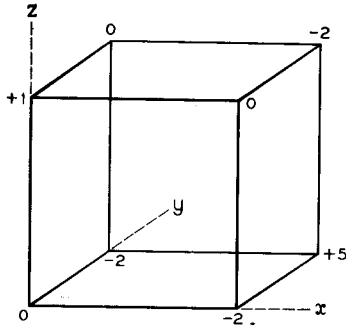


Fig. 2 — A period of the periodic function.

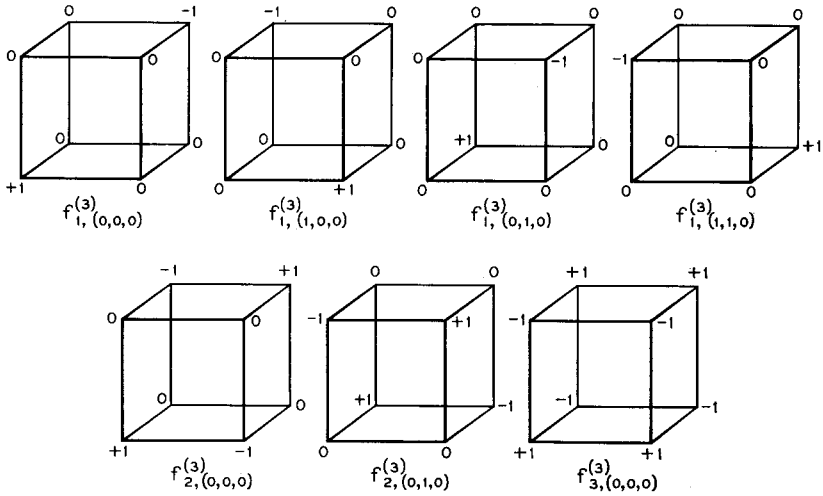


FIG. 3 — The seven basis functions.

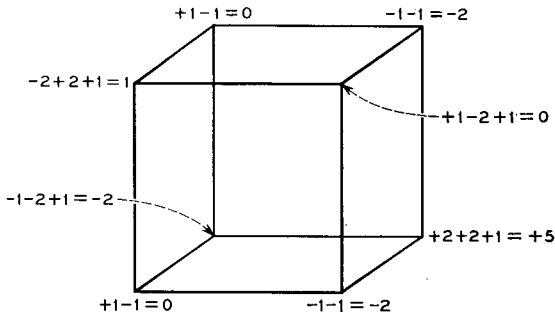


Fig. 4 — Decomposition of the periodic function.

The coefficient of $f_{1,(0,0,0)}^{(3)}$ is obviously $\frac{1}{2}(0 - (-2)) = 1$, etc., so that we obtain

$$f = f_{1,(0,0,0)}^{(3)} - f_{1,(1,0,0)}^{(3)} - f_{1,(0,1,0)}^{(3)} \\ + 2f_{1,(1,1,0)}^{(3)} - 2f_{2,(0,1,0)}^{(3)} - f_{3,(0,0,0)}^{(3)}$$

Graphically, this equality is shown in Fig. 4.

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