

A Comparison of the Q -Functions and the Translation Function of Crowther and Blow

BY PATRICK TOLLIN

Carnegie Laboratory of Physics, University of Dundee, Dundee, Scotland

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An attempt is made to show that the Q -functions [Tollin, *Acta Cryst.* (1966) **21**, 613] and the translation function [Crowther & Blow, *Acta Cryst.* (1967) **23**, 544] are virtually identical, and the modifications to the translation function proposed by Crowther & Blow are discussed.

The translation problem is the problem of determining the position in the unit cell of a known molecule, or known part of a molecule, once its orientation with respect to the crystal axes has been determined. A number of solutions to this problem have been proposed (Nordman & Nakatsu, 1963; Vand & Pepinsky, 1956; Hoppe, 1957; Huber, 1965 and others). In particular Tollin & Cochran (1964) (hereafter TC) proposed a set of functions, which they called Q -functions, which made use of the properties of the sum function (Buerger, 1959). Later Tollin (1966*a*) (hereafter PT) proposed a modification of these Q -functions which allowed the determination of the position of the known group with respect to the individual symmetry elements of the space group of the crystal, in turn. Subsequently Crowther & Blow (1967) (hereafter CB) proposed a new solution to the translation function. The object of this note is to show that the Q -functions and the translation function of CB are virtually identical. That the close similarity between these two functions is not immediately obvious is a result firstly of the different notations used by the authors and secondly of the fact that in PT the Q -functions have been expressed in terms of the sum function while the translation function of CB is explained in terms of the Patterson function.

The translation function $T(\mathbf{t})$, which has its largest value when \mathbf{t} is the vector between two molecules related by a symmetry element, is defined in CB by the equation:

$$T(\mathbf{t}) = \sum_{\mathbf{h}} |F(\mathbf{h})|^2 F_m(\mathbf{h}) F_m^*(\mathbf{h} \cdot \mathbf{A}) \exp(-2\pi i \mathbf{h} \cdot \mathbf{t}).$$

$|F(\mathbf{h})|$ are the observed structure amplitudes and $F_m(\mathbf{h})$ are the structure factors of the known group with respect to the local origin. The particular symmetry operation of the space group relates the point defined by the vector \mathbf{x} to the point $\mathbf{A} \cdot \mathbf{x} + \mathbf{d}$. If there are n atoms in the known group having coordinates \mathbf{r}_j with respect to the arbitrary origin, whose position in the unit cell is \mathbf{s}_0 , then

$$F_m(\mathbf{h}) = \sum_{j=1}^n f_j \exp(+2\pi i \mathbf{h} \cdot \mathbf{r}_j) = C + iS.$$

If, for the present, we ignore the scattering factors f_j , then the translation function can be written

$$T(\mathbf{t}) = \sum_{\mathbf{h}} |F(\mathbf{h})|^2 \sum_{j=1}^n \sum_{j'=1}^n \cos [2\pi \mathbf{h} \cdot (\mathbf{r}_j - \mathbf{A} \cdot \mathbf{r}_{j'} - \mathbf{t})].$$

In PT the vector \mathbf{R}_0 is defined as the vector which fixes the arbitrary origin with respect to the symmetry element and not the origin of the unit cell, it is convenient therefore at present to ignore the vector \mathbf{d} . Since, in the notation of CB

$$\mathbf{t} = \mathbf{A} \cdot \mathbf{s} - \mathbf{s}$$

(CB Fig. 1), the above equation for $T(\mathbf{t})$ can be written

$$T(\mathbf{s}) = \sum_{\mathbf{h}} |F(\mathbf{h})|^2 \sum_{j,j'=1}^n \cos \{2\pi \mathbf{h} \cdot [\mathbf{r}_j + \mathbf{s} - \mathbf{A} \cdot (\mathbf{r}_{j'} + \mathbf{s})]\},$$

which is identical with the expression for $Q(\mathbf{R}_0)$ given in equation (2) of PT. Introducing the vector \mathbf{d} merely shifts the origin of the function and corresponds to defining the vector \mathbf{R}_0 as the vector from the origin of the unit cell to the local origin as in TC. Introducing the scattering factors f_j corresponds to replacing the sum function, equation (1) of PT, by the alpha-synthesis (Ramachandran & Raman, 1959) and, as they show, this gives peaks in the same positions as the sum function, and, unless atoms of the structure have markedly different scattering powers, does not make a great difference to the function.

The identity of the two methods is also seen by considering the section of $T(t_x t_y t_z)$ at $t_y = \frac{1}{2}$ in the last paragraph of CB. Then,

$$\begin{aligned} T(t_x, \frac{1}{2}, t_z) &= \sum_{\mathbf{h}} \sum_k \sum_l (-1)^k |F(hkl)|^2 \\ &\times \{ [C(hkl)C(h\bar{k}l) - S(hkl)S(h\bar{k}l)] \cos 2\pi(ht_x + lt_z) \\ &- [C(hkl)S(h\bar{k}l) + C(h\bar{k}l)S(hkl)] \sin 2\pi(ht_x + lt_z) \}, \end{aligned}$$

which is identical with the expression for $Q(X_0 Z_0)$ of PT.

Two modified translation functions are proposed by CB. The expression which they suggest for $T_2(\mathbf{t})$, which is the translation function obtained by considering all the symmetry operations simultaneously, bears a close resemblance to the original $Q(\mathbf{r}_0)$ defined in TC, where the point is made that 'when \mathbf{r}_0 has its correct value, the value of $Q(\mathbf{r}_0)$ is simply the sum of the values of the Patterson function at positions which correspond to vectors between atoms in different groups.' The function $T_1(\mathbf{t})$ defined in CB makes use of the Patterson

function after the origin peak and the intramolecular vectors have been removed. This corresponds to an extension of the point made in PT that the origin peak may lead to false peaks in the Q -function, but can be removed.

The expression for $T(\mathbf{t})$ obtained by CB represents in one respect a more general form of the Q -functions than that given by PT. Since $T(\mathbf{t})$ is expressed in terms of $F_m(\mathbf{h})$, the transform of the individual molecule, it need not be calculated, as suggested by the expressions given above, in terms of a set of discrete atoms. If, for example, a molecule of a protein has been obtained at less than atomic resolution, its transform may still be calculated by numerical methods from the electron density. The possibility of such an extension has been suggested previously (Tollin, 1966*b*) in terms of the Q -functions. In this case the quantities CC' and SS' in the notation of PT must be obtained by such numerical integration. At what resolution such a function will prove useful is a matter for experiment.

The Q -functions have now been successfully applied to the determination of the structure of a number of molecular crystals (for example, Young, Tollin & Sutherland, 1968; Tollin, Young & Wilson, 1968). Recently the author has applied the Q -function to the determination of the position in the unit cell of the seal myoglobin molecule (Scouloudi, 1960) once its orientation had been determined. The orientation was found using the rotation function (Rossmann & Blow, 1962) to compare the 5.8 Å resolution data for seal and sperm whale myoglobin (Tollin, 1966*b*). A report of the details of this determination is in preparation. However, it is worth noting here that since the protein molecule is so large that many atoms are in positions

which would give rise to non-Harker peaks in the Harker section, it is essential in this case to remove the origin peak from the Patterson.

It should be noted that, as Hoppe & Paulus (1967) mention in a footnote, 'it is possible to translate operations with convolution molecules into reciprocal space. . .'. The Q -functions are closely similar to the reciprocal space equivalent of the convolution molecule method where the sum of the convolution molecule and the Patterson structure is used as the criterion of fit.

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A Contribution to the Dynamical Diffraction Theory of Scalar Waves in Crystals

By P. HUISMÄKI

Department of Technical Physics, Technical University of Helsinki, Otaniemi, Finland

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A matrix formalism is developed for calculating the elastically scattered waves diffracted by an infinite plane parallel crystal. Introduction of projection operators makes it possible to cover both Laue and Bragg reflected waves under the same formalism.

1. Introduction

The basic problem to be considered is the solving of the time-independent Schrödinger equation

$$(\nabla^2 + k^2)\psi(\mathbf{r}) = u(\mathbf{r})\psi(\mathbf{r}) \quad (1.1)$$

for a potential $V(\mathbf{r}) = (\hbar^2/2\mu)u(\mathbf{r})$, periodic inside a three-dimensional crystal lattice and zero outside. k is the

wave number and μ the mass of the particle associated with the scalar field $\psi(\mathbf{r})$. In diffraction experiments an incident wave falls upon the crystal and an outgoing wave scattered by the crystal is detected. This is described more adequately by the integral equation

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) - \frac{1}{4\pi} \int_V \frac{\exp ik|\mathbf{r}-\mathbf{r}'|}{|\mathbf{r}-\mathbf{r}'|} u(\mathbf{r}')\psi(\mathbf{r}')d^3\mathbf{r}' \quad (1.2)$$