

1.3. Fourier transforms in crystallography: theory, algorithms and applications

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1.3.1. General introduction

Since the publication of Volume II of *International Tables*, most aspects of the theory, computation and applications of Fourier transforms have undergone considerable development, often to the point of being hardly recognizable.

The mathematical analysis of the Fourier transformation has been extensively reformulated within the framework of distribution theory, following Schwartz's work in the early 1950s.

The computation of Fourier transforms has been revolutionized by the advent of digital computers and of the Cooley–Tukey algorithm, and progress has been made at an ever-accelerating pace in the design of new types of algorithms and in optimizing their interplay with machine architecture.

These advances have transformed both theory and practice in several fields which rely heavily on Fourier methods; much of electrical engineering, for instance, has become digital signal processing.

By contrast, crystallography has remained relatively unaffected by these developments. From the conceptual point of view, old-fashioned Fourier series are still adequate for the quantitative description of X-ray diffraction, as this rarely entails consideration of molecular transforms between reciprocal-lattice points. From the practical point of view, three-dimensional Fourier transforms have mostly been used as a tool for visualizing electron-density maps, so that only moderate urgency was given to trying to achieve ultimate efficiency in these relatively infrequent calculations.

Recent advances in phasing and refinement methods, however, have placed renewed emphasis on concepts and techniques long used in digital signal processing, *e.g.* flexible sampling, Shannon interpolation, linear filtering, and interchange between convolution and multiplication. These methods are iterative in nature, and thus generate a strong incentive to design new crystallographic Fourier transform algorithms making the fullest possible use of all available symmetry to save both storage and computation.

As a result, need has arisen for a modern and coherent account of Fourier transform methods in crystallography which would provide:

(i) a simple and foolproof means of switching between the three different guises in which the Fourier transformation is encountered (Fourier transforms, Fourier series and discrete Fourier transforms), both formally and computationally;

(ii) an up-to-date presentation of the most important algorithms for the efficient numerical calculation of discrete Fourier transforms;

(iii) a systematic study of the incorporation of symmetry into the calculation of crystallographic discrete Fourier transforms;

(iv) a survey of the main types of crystallographic computations based on the Fourier transformation.

The rapid pace of progress in these fields implies that such an account would be struck by quasi-immediate obsolescence if it were written solely for the purpose of compiling a catalogue of results and formulae 'customized' for crystallographic use. Instead, the emphasis has been placed on a mode of presentation in which most results and formulae are *derived* rather than listed. This does entail a substantial mathematical overhead, but has the advantage of preserving in its 'native' form the context within which these results are obtained. It is this context, rather than any particular set of results, which constitutes the most fertile source

of new ideas and new applications, and as such can have any hope at all of remaining useful in the long run.

These conditions have led to the following choices:

(i) the mathematical theory of the Fourier transformation has been cast in the language of Schwartz's theory of distributions which has long been adopted in several applied fields, in particular electrical engineering, with considerable success; the extra work involved handsomely pays for itself by allowing the three different types of Fourier transformations to be treated together, and by making all properties of the Fourier transform consequences of a single property (the convolution theorem). This is particularly useful in all questions related to the sampling theorem;

(ii) the various numerical algorithms have been presented as the consequences of basic algebraic phenomena involving Abelian groups, rings and finite fields; this degree of formalization greatly helps the subsequent incorporation of symmetry;

(iii) the algebraic nature of space groups has been re-emphasized so as to build up a framework which can accommodate both the phenomena used to factor the discrete Fourier transform and those which underlie the existence (and lead to the classification) of space groups; this common ground is found in the notion of *module over a group ring* (*i.e.* integral representation theory), which is then applied to the formulation of a large number of algorithms, many of which are new;

(iv) the survey of the main types of crystallographic computations has tried to highlight the roles played by various properties of the Fourier transformation, and the ways in which a better exploitation of these properties has been the driving force behind the discovery of more powerful methods.

In keeping with this philosophy, the theory is presented first, followed by the crystallographic applications. There are 'forward references' from mathematical results to the applications which later invoke them (thus giving 'real-life' examples rather than artificial ones), and 'backward references' as usual. In this way, the internal logic of the mathematical developments – the surest guide to future innovations – can be preserved, whereas the alternative solution of relegating these to appendices tends on the contrary to obscure that logic by subordinating it to that of the applications.

It is hoped that this attempt at an overall presentation of the main features of Fourier transforms and of their ubiquitous role in crystallography will be found useful by scientists both within and outside the field.

1.3.2. The mathematical theory of the Fourier transformation

1.3.2.1. Introduction

The Fourier transformation and the practical applications to which it gives rise occur in three different forms which, although they display a similar range of phenomena, normally require distinct formulations and different proof techniques:

(i) *Fourier transforms*, in which both function and transform depend on continuous variables;

(ii) *Fourier series*, which relate a periodic function to a discrete set of coefficients indexed by n -tuples of integers;

(iii) *discrete Fourier transforms*, which relate finite-dimensional vectors by linear operations representable by matrices.