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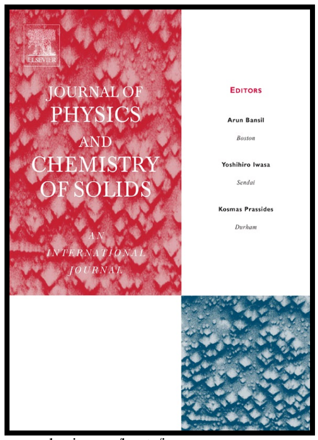

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G. Kontrym-Sznajd, A. Holas

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Lattice harmonics expansion revisited

G. Kontrym-Sznajd[a,*], A. Holas[b]

[a] Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, 50-422 Wrocław, Poland
[b] Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01–224 Warsaw, Poland

Abstract

The main subject of the work is to provide the most effective way of determining the expansion of some quantities into orthogonal polynomials, when these quantities are known only along some limited number of sampling directions. By comparing the commonly used Houston method with the method based on the orthogonality relation, some relationships, which define the applicability and correctness of these methods, are demonstrated. They are verified for various sets of sampling directions applicable for expanding quantities having the full symmetry of the Brillouin zone of cubic and non-cubic lattices. All results clearly show that the Houston method is always better than the orthogonality-relation one. For the cubic symmetry we present a few sets of special directions (SDs) showing how their construction and, next, a proper application depend on the choice of various sets of lattice harmonics. SDs are important mainly for experimentalists who want to reconstruct anisotropic quantities from their measurements, performed at a limited number of sampling directions.

Keywords: lattice harmonics, expansion methods, special directions, Brillouin zone sampling

1. Introduction

In crystals, various physical quantities, both in the real and reciprocal spaces, are invariant under transformations of the point group of the crystal. Let $f(\boldsymbol{p})$ denotes such a quantity, a function of the vector $\boldsymbol{p} = (p, \theta, \phi) = p\,(\sin(\theta)\cos(\phi), \sin(\theta)\sin(\phi), \cos(\theta))$ (in spherical and cartesian coordinates, respectively), belonging to a particular space. For many applications it is convenient to express this function as an expansion into a series of lattice harmonics $F_{l,\nu}(\theta,\phi)$ of an appropriate symmetry[1]:

$$f(\boldsymbol{p}) = f(p,\theta,\phi) = \sum_{l,\nu} f_{l,\nu}(p)\, F_{l,\nu}(\theta,\phi)\,, \tag{1}$$

where the index ν distinguishes harmonics of the same order l. Due to the orthogonality of the lattice harmonics, $f_{l,\nu}(p)$ are expressed by the integrals:.

$$f_{l,\nu}(p) = \int f(p,\theta,\phi)\, F_{l,\nu}(\theta,\phi)\, \sin(\theta)\, \mathrm{d}\theta\, \mathrm{d}\phi \tag{2}$$

The use of the notation "$\boldsymbol{p}$" is connected with the fact that we consider quantities in the momentum space in which screw-rotation axes and glide-reflection planes are replaced by rotation axes and reflection planes. Moreover, our considerations are restricted to quantities having the full symmetry of the Brillouin zone, for example, the electron momentum density, the Fermi surface, the effective mass, and others. Of course, the mentioned expansion is valid also in the real space if harmonics are the same (i.e. except crystals described by non-symmorphic groups). What are the benefits of the lattice harmonics expansion? Apart from the fact that theoretical calculations (the same concerns experimental investigations) are limited to the irreducible part of the Brillouin zone (or the Wigner-Seitz cell), knowledge of the expansion coefficients $f_{l,\nu}(p)$ allows to determine values of $f(\boldsymbol{p})$ at an arbitrary point $\boldsymbol{p}$. Of course, the quantity $f(\boldsymbol{p})$ is reasonably described by Eq. (1) if the series is well convergent and sufficiently accurate when limited to some finite number of the lattice harmonics. Here it should be pointed out that, in order to estimate properly a few components $f_{l,\nu}(p)$ from knowledge of $f(\boldsymbol{p})$ along a few sampling directions, one should use very particular directions of $\boldsymbol{p}$, the so-called special directions (SDs), proposed for the first time by Bansil [2].

The expansion into lattice harmonics (or into spherical harmonics in the absence of a symmetry) has also other very important applications. It allows for analyti-

*Corresponding author tel.: +48 71 3954 131
Email address: g.sznajd@int.pan.wroc.pl (G. Kontrym-Sznajd)