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WREATH GROUPS AND DIFFRACTION INTENSITY SYMMETRY

Daniel B. Litvin
Eberly College of Science
The Pennsylvania State University
Penn State Berks, P.O. Box 7009, Reading, PA 19610-6009, USA
e-mail: u3c@psu.edu

Abstract: Wreath product groups are defined in reciprocal space which give rise to symmetry groups of the diffraction intensity of both periodic crystals and quasicrystals.

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1. Introduction

The x-ray diffraction intensity function I of a crystalline or quasicrystalline material depends on the components, i.e. values, of the reciprocal space density function ρ, the Fourier transform of the real space density function P. That is

$$I(\mathbf{k}) = |\rho(\mathbf{k})|^2 \tag{1}$$

and

$$P(\mathbf{r}) = \sum_{\mathbf{k}} \rho(\mathbf{k}) \mathbf{e}^{2\pi i \mathbf{k}\cdot\mathbf{r}} . \tag{2}$$

The summation in the latter is over a finitely generated, but not necessarily discrete, set of reciprocal vectors $\mathbf{k}$ determined by the diffraction intensity.

When speaking of a symmetry of the diffraction intensity $I(\mathbf{k})$ we shall mean an operation $[g]$ defined to act on a diffraction intensity function I such that the values of the functions I and $[g]I$ are related by

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$$[g]I(\mathbf{k}) = I(g^{-1}\mathbf{k}) \tag{3}$$

and which leave the diffraction intensity function invariant:

$$[g]I(\mathbf{k}) = I(\mathbf{k})\,. \tag{4}$$

Let $[O]$ be an operator which acts on the reciprocal space density function ρ. If

$$\mid [O]\rho(\mathbf{k}) \mid^2 = [g]I(\mathbf{k}) \tag{5}$$

we shall say that the operator $[O]$ of the reciprocal space density function ρ gives rise to or is related to the operator $[g]$ of the diffraction intensity function I. In this paper we shall be interested in defining operators $[O]$ which give rise to operators $[g]$ acting on the diffraction intensity function I which are symmetries of the diffraction intensity function:

$$\mid [O]\rho(\mathbf{k}) \mid^2 = [g]I(\mathbf{k}) = I(\mathbf{k})\,. \tag{6}$$

In Section 2 we introduce operators which are defined to act on the function ρ. The wreath product groups of such reciprocal space operators which give rise to symmetries of the diffraction intensity function are defined in Section 3. In Section 4 we show how these wreath product groups are related to the reciprocal space symmetry appproach to the study of crystals [1] and quasicrystals [5].

2. Operators Acting on the Reciprocal Space Density Function ρ

The function ρ is a mapping $K \to \mathfrak{C}$ from the set K of reciprocal vectors into the set $\mathfrak{C}$ consisting of the field of complex numbers. This function will be denoted here by $\rho = \{\mathbf{k}, \rho(\mathbf{k})\}$ denoting the complex number $\rho(\mathbf{k})$ of $\mathfrak{C}$ into which the element $\mathbf{k}$ of the set K is mapped. Let $U_{K\mathfrak{C}}$ denote the set of all functions ρ from K into $\mathfrak{C}$. An operator acting on a function ρ of the set $U_{K\mathfrak{C}}$ is defined as an element of the direct product group $\mathbf{S}(\mathbf{k})x\mathbf{S}(\mathfrak{C})$, where $\mathbf{S}(\mathbf{k})$ is the symmetric group of the set K and $\mathbf{S}(\mathfrak{C})$ the symmetric group of the set $\mathfrak{C}$. An element of this direct product group will be denoted by $[g \mid q]$, where g is a permutation of the set K and q a permutation of the set $\mathfrak{C}$.

Let e denote the identity permutation. The action of an operator $[g \mid e]$ on a function ρ is then given by:

$$[g \mid e]\rho = [g \mid e]\{\mathbf{k}, \rho(\mathbf{k})\} = \{g\mathbf{k}, \rho(\mathbf{k})\} = \{\mathbf{k}, \rho(g^{-1}\mathbf{k})\}\,. \tag{7}$$

That is, the function $[g \mid e]\rho$ maps the element $\mathbf{k}$ of K into the complex number which the function ρ maps the element $g^{-1}\mathbf{k}$. In terms of the values of the functions ρ and $[g \mid e]\rho$, the value of the function $[g \mid e]\rho$ at $\mathbf{k}$ is equal to the value of the function ρ at $g^{-1}\mathbf{k}$, i.e.:

$$[g \mid e]\rho(\mathbf{k}) = \rho(g^{-1}\mathbf{k})\,. \tag{8}$$

The action of an operator $[e \mid q]$ on a function ρ is given by:

$$[e \mid q]\rho = [e \mid q]\{\mathbf{k}, \rho(\mathbf{k})\} = \{\mathbf{k}, (q\rho)(\mathbf{k})\}\,. \tag{9}$$

In terms of the values of the functions ρ and $[e \mid q]\rho$:

$$[e \mid q]\rho(\mathbf{k}) = q\rho(\mathbf{k})\,. \tag{10}$$

That is, the value of the function $[e \mid q]\rho$ at $\mathbf{k}$ is equal to the value into which the value of the function ρ at $\mathbf{k}$ is permuted by the permutation q.

The action of an operator $[g \mid q]$ on a function ρ is given by

$$[g \mid q]\rho = [g \mid q]\{\mathbf{k}, \rho(\mathbf{k})\} = \{g\mathbf{k}, (q\rho)(\mathbf{k})\} = \{\mathbf{k}, (q\rho)(g^{-1}\mathbf{k})\} \tag{11}$$

and in terms of the values of the functions ρ and $[g \mid q]\rho$:

$$[g \mid q]\rho(\mathbf{k}) = q\rho(g^{-1}\mathbf{k})\,. \tag{12}$$

Since

$$[g \mid q_g][h \mid q_h]\rho = [g \mid q_g]\{h\mathbf{k}, q_h\rho(\mathbf{k})\} = \{gh\mathbf{k}, q_g q_h \rho(\mathbf{k})\}\,, \tag{13}$$

or in terms of the values of the functions

$$\begin{aligned}[g \mid q_g][h \mid q_h]\rho(\mathbf{k}) = q_g[h \mid q_h]\rho(g^{-1}\mathbf{k}) &= q_g q_h \rho(h^{-1}g^{-1}\mathbf{k}) \\ &= q_g q_h \rho((gh)^{-1}\mathbf{k})\,,\end{aligned} \tag{14}$$

the product of two such operators is given by:

$$[g \mid q_g][h \mid q_h] = [gh \mid q_g q_h]\,. \tag{15}$$

Operators $[g \mid q]$ defined to act on a function ρ, see equations (11) and (12), are not the most general operators which can be defined, see [7]. In an operator $[g \mid q]$, the permutation g is coupled to a single permutation q of the symmetric group $\mathbf{S}(\mathfrak{C})$ and this single permutation acts, see equation (11), on every value $\rho(\mathbf{k})$ of the function ρ. One can generalize this type of operator by defining a function coupled to the permutation g in a manner that the operator can then act via a different permutation of $\mathbf{S}(\mathfrak{C})$ on values of the function ρ mapped from different reciprocal vectors $\mathbf{k}$.

Let Φ be a mapping $K \to \mathbf{S}(\mathfrak{C})$ of the set K of reciprocal vectors into the symmetric group $\mathbf{S}(\mathfrak{C})$ of the field of complex numbers, i.e. $\Phi = \{\mathbf{k}, \mathbf{q}(\mathbf{k})\}$, where $\mathbf{q}(\mathbf{k})$ is the permutation of $\mathbf{S}(\mathfrak{C})$ into which the reciprocal vector $\mathbf{k}$ is mapped. We construct operators $[g \mid \Phi]$, pairs consisting of a permutation g of $\mathbf{S}(\mathbf{k})$ and a function Φ, which are defined to act on the function ρ by

$$[g \mid \Phi]\rho = [g \mid \Phi]\{\mathbf{k}, \rho(\mathbf{k})\} = \{g\mathbf{k}, (q(\mathbf{k})\rho)(\mathbf{k})\} = \{\mathbf{k}, (q(g^{-1}\mathbf{k})\rho)(g^{-1}\mathbf{k})\}\,. \tag{16}$$

In terms of the values of the function ρ, this is:

$$[g \mid \Phi]\rho(\mathbf{k}) = q(g^{-1}\mathbf{k})\rho)(g^{-1}\mathbf{k})\,. \tag{17}$$

The value of the function $[g \mid \Phi]\rho$ at $\mathbf{k}$ is equal to the value of the function ρ at $g^{-1}\mathbf{k}$ permuted by the permutation $q(g^{-1}\mathbf{k})$ into which the reciprocal vector $g^{-1}\mathbf{k}$ is mapped by Φ. Since

$$\begin{aligned}[g \mid \Phi_g][h \mid \Phi_h]\rho &= [g \mid \Phi_g][h \mid \Phi_h]\{\mathbf{k}, \rho(\mathbf{k})\} \\ &= [g \mid \Phi_g]\{h\mathbf{k}, (q_h(\mathbf{k})\rho)(\mathbf{k})\} = \{gh\mathbf{k}, q_g(h\mathbf{k})(q_h(\mathbf{k})\rho)(\mathbf{k})\}\,,\end{aligned} \tag{18}$$

or in terms of the values of the function

$$\begin{aligned}&[g \mid \Phi_g][h \mid \Phi_h]\rho(\mathbf{k}) = q_g(g^{-1}\mathbf{k})[h \mid \Phi_h]\rho(g^{-1}\mathbf{k}) \\ &= q_g(g^{-1}\mathbf{k})q_h(h^{-1}g^{-1}\mathbf{k})\rho(h^{-1}g^{-1}\mathbf{k}) = q_g(g^{-1}\mathbf{k})q_h((gh)^{-1}\mathbf{k})\rho((gh)^{-1}\mathbf{k})\end{aligned} \tag{19}$$

the product of two such operators is

$$[g \mid \Phi_g][h \mid \Phi_h] = [gh \mid \Phi_{gh}]\,, \tag{20}$$

where Φ_{gh} maps each reciprocal vector $\mathbf{k}$ into the permutation

$$q_{gh}(\mathbf{k}) = q_g(h\mathbf{k})q_h(\mathbf{k}) \tag{21}$$

of $\mathbf{S}(\mathfrak{C})$. A group of such operations, defined in equations (16) and (17), is known as a wreath product group [7]. If each of the mappings Φ_g are mappings onto a single permutation q of $\mathbf{S}(\mathfrak{C})$, i.e. is independent of $\mathbf{k}$, then the wreath group becomes a group of operators $[g \mid q]$ as defined in equations (11) and (12).

3. Operators of ρ vis-à-vis symmetries of I

To determine operators $[g \mid \Phi_g]$ of the reciprocal space density function ρ which give rise to symmetries, equation (4), of the diffraction intensity function I requires that

$$\mid [g \mid \Phi_g]\rho(\mathbf{k}) \mid^2 = [g]I(\mathbf{k})\,, \tag{22}$$

that is, using equations (3) and (17)

$$\mid q(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k}) \mid^2 = \mid \rho(g^{-1}\mathbf{k}) \mid^2\,, \tag{23}$$

where $q(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k})$ denotes the complex number which is the image of the complex number $\rho(g^{-1}\mathbf{k})$ under the permutation $q(g^{-1}\mathbf{k})$ of $\mathbf{S}(\mathfrak{C})$. Since both $q(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k})$ and $\rho(g^{-1}\mathbf{k})$ are complex numbers, there exists a third complex number $c(g^{-1}\mathbf{k})$ such that

$$q(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k}) = c(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k}) \tag{24}$$

and equation (23) becomes:

$$| c(g^{-1}\mathbf{k}) |^2 | \rho(g^{-1}\mathbf{k}) |^2 = | \rho(g^{-1}\mathbf{k}) |^2 \ . \tag{25}$$

Consequently, operators $[g \mid \Phi_g]$ of the reciprocal space density function ρ which give reise to symmetries $[g]$ of the diffraction intensity function I are those with mappings Φ_g having corresponding complex numbers $c(g^{-1}\mathbf{k})$ defined by equation (24) which satisfy equation (25). That is, each complex number $c(g^{-1}\mathbf{k})$ satisfies:

$$| c(g^{-1}\mathbf{k}) |^2 = 1 \, . \tag{26}$$

We shall denote such symmetries $[g \mid \Phi_g]$ of ρ as $[g \mid c_g(\mathbf{k})]$. In this notation, the action of the operator on ρ, equation (16), is written as:

$$\begin{aligned}[g \mid c_g(\mathbf{k})]\rho &= [g \mid c_g(\mathbf{k})]\{\mathbf{k}, \rho(\mathbf{k})\} \\ &= \{g\mathbf{k}, c_g(\mathbf{k})\rho(\mathbf{k})\} = \{\mathbf{k}, c_g(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k})\} \, .\end{aligned} \tag{27}$$

In terms of the values of the function ρ, equation (17) is written as

$$[g \mid c_g(\mathbf{k})]\rho(\mathbf{k}) = c_g(g^{-1}\mathbf{k})\rho(g^{-1}\mathbf{k}) \tag{28}$$

and the product of two operators, equation (20) as

$$[g \mid c_g(\mathbf{k})][h \mid c_h(\mathbf{k})] = [gh \mid c_{gh}(\mathbf{k})] \, , \tag{29}$$

where:

$$c_{gh}(\mathbf{k}) = c_g(h\mathbf{k})c_h(\mathbf{k}) \, . \tag{30}$$

We have then derived operators $[O] = [g \mid c_g(\mathbf{k})]$ which give rise to symmetries, equations (4) and (22), of the diffraction intensity function I.

We have considered only operators in reciprocal space which give rise to symmetries of the diffraction intensity function relating intensities of the same magnitude. From equations (3) and (4)

$$[g]I(\mathbf{k}) = I(g^{-1}\mathbf{k}) = I(\mathbf{k}) \tag{31}$$

and operators $[g]$ relate diffraction intensities at points of equal magnitude. We note that the concept of symmetry of the diffraction intensity function can be expanded to include symmetries which relate intensities of different magnitude. One can define operators $[g \mid R_g(\mathbf{k})]$ [4], where $R_g(\mathbf{k})$ is a function whose values are real, defined to act on the diffraction intensity function as

$$[g \mid R_g(\mathbf{k})]I(\mathbf{k}) = R_g(\mathbf{k})I(g^{-1}\mathbf{k}) \tag{32}$$

and which leave the intensity function invarinat. Such symmetries of the diffraction intensity function are related to symmetries $[g \mid c_g(\mathbf{k})]$ of the reciprocal space density function, where $| c_g(\mathbf{k}) |^2 = R_g(\mathbf{k})$.

4. Relation to Reciprocal Space Symmetry of Periodic Crystals and Quasicrystals

Since the complex numbers $c_g(\mathbf{k})$ of the operators $[g \mid c_g(\mathbf{k})]$ satisfy equation (26), one can rewrite them in the format:

$$c_g(\mathbf{k}) = \mathbf{e}^{2\pi i \Omega_g(\mathbf{k})} . \tag{33}$$

Using this notation, equation (27) and the product, equation (30), can be rewritten as

$$\rho(g\mathbf{k}) = \mathbf{e}^{2\pi i \Omega_g(\mathbf{k})} \rho(\mathbf{k}) \tag{34}$$

and

$$\Omega_{gh}(\mathbf{k}) = \Omega_g(h\mathbf{k}) + \Omega_h(\mathbf{k}) . \tag{35}$$

These later two equations are used to define reciprocal space operators of quasicrystals by Rokhsar, Wright, and Mermin [8], Lifshitz [3], Mermin [6], and Fisher and Robson [2]. The special case of a discrete set of reciprocal $\mathbf{k}$ vectors and functions $\Omega_g(\mathbf{k}) = \mathbf{k}\cdot\tau_g$, where τ_g is a vector independent of $\mathbf{k}$, was used to describe the reciprocal space operators of periodic crystals by Bienenstock and Ewald [1].

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