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ON GROUP STRUCTURE IN COPERNICAN QUASICRYSTALLOGRAPHY*

B. Baumgartner, M. Breitenecker and H. Urbantke

Institut für Theoretische Physik, Universität Wien
Boltzmanngasse 5, 1090 Wien, Austria

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Dedicated to Andrzej Trautman in honour of his 64^{th} birthday

The group structure of quasicrystallographic space groups is described in an alternative way, using the language of group extensions. The rôle of the lattice of translations in classical crystallography is pointed out to be taken by the *abstract* dual of the generalized kind of lattice in Fourier space that one has in the quasi case.

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1. Introduction

In their 'Copernican' [1] approach to quasicrystallography, N.D. Mermin and coworkers specify space groups by their point groups and certain associated phase functions. In the main body of these works, the group structure of these objects is not manifest, and they are given such structure only in an appendix to [2]. In the present note we give an alternative description of this structure that closely parallels an alternative description of the space groups of classical crystallography as group extensions, given by cocycles on the point group with values in the *abstract* dual of the (generalized) lattice Λ in Fourier space.

2. Standard crystallographic situation

Here one has the Euclidean group E(3)of motions in real physical 3–space with its subgroups T(3) of translations and O(3) of rotations and reflections.

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Thus there is the splitting exact sequence [3]

$$0 \to \mathrm{T}(3) \to \mathrm{E}(3) \;\rightleftarrows\; \mathrm{O}(3) \to 1.$$

A crystallographic space group $\mathcal{G}$ is a discrete subgroup of E(3) with its lattice $\mathcal{T}$ of translations and the finite 'point group' $\mathcal{G}_0 \subset \mathrm{O}(3)$ leaving the lattice $\mathcal{T}$ invariant; but in general, the exact sequence [3]

$$0 \to \mathcal{T} \to \mathcal{G} \to \mathcal{G}_0 \to 1$$

does not split. (If it does, $\mathcal{G}$ is called 'symmorphic' by crystallographers.) In mathematics, in this situation $\mathcal{G}$ is called [4, 5] an *extension* of $\mathcal{G}_0$ by the (abelian) group $\mathcal{T}$ — or an extension of $\mathcal{T}$ by $\mathcal{G}_0$, according to others [6] — and it is shown there that such an extension is characterized by *(i)* a homomorphism of $\mathcal{G}_0$ into Aut $\mathcal{T}$ (the group of automorphisms of $\mathcal{T}$) and *(ii)* by a *cocycle* on $\mathcal{G}_0$ with values in $\mathcal{T}$ (if $\mathcal{T}$ is abelian as it is in our case). This means that the above exact sequence of groups, and the group $\mathcal{G}$ in particular, may be reconstructed abstractly from $\mathcal{T}$, $\mathcal{G}_0$, its action on $\mathcal{T}$, and an extension cocycle, by a textbook procedure [4–6].

3. Quasicrystallographic situation

In 'Copernican' (quasi)crystallography, one starts with a finitely generated free $\boldsymbol{Z}$–module $\Lambda \subset \boldsymbol{R}^3$ (which generalizes the reciprocal lattice of standard crystals and which, in the quasi case, has more than 3 free generators, so that it may even be dense in $\boldsymbol{R}^3$) together with a point group $\mathcal{G}_0 \subset O(3)$ leaving Λ invariant. To specify a space group belonging to $\mathcal{G}_0$, Λ, one has to write down a real–valued phase function Φ_g on Λ for each $g \in \mathcal{G}_0$, $\boldsymbol{Z}$–linear when reduced mod $\boldsymbol{Z}$, such that the following 'group compatibility condition'[1] holds:

$$z_{g,g'} := \Phi_g - \Phi_{gg'} + g\Phi_{g'} \in \boldsymbol{Z}^{\Lambda}\,, \qquad \text{all } g, g' \in \mathcal{G}_0\,.$$

Here $\boldsymbol{Z}^{\Lambda}$ is the $\boldsymbol{Z}$–module of integer–valued functions on Λ, addition and subtraction are pointwise, and the action of $\mathcal{G}_0$ on functions Φ from Λ to $\boldsymbol{R}$ or $\boldsymbol{Z}$ is given by $(g\Phi)(k) = \Phi(g^{-1}k)$, $k \in \Lambda$. Now the first point to make is that z is a 2–cocycle on $\mathcal{G}_0$ with values in the abelian group $\boldsymbol{Z}^{\Lambda}$ with respect to the action of $\mathcal{G}_0$ just defined. This is to say that z satisfies the cocycle condition

$$gz_{g',g''} - z_{gg',g''} + z_{g,g'g''} - z_{g,g'} = 0\,, \qquad \text{all} g, g', g'' \in \mathcal{G}_0\,.$$

[1] The slight difference between Mermin's form of this condition and ours arises because we call Φ_g what he would write $\Phi_{g^{-1}}$. This is to conform with the *left* action of $\mathcal{G}_0$ on $\mathbf{Z}^{\Lambda}$ as given in the following.

We assume that the Φ_g are gauged [7] such that $\Phi_e = 0$ (whence $z_{e,g} = 0 = z_{g,e}$), e being the unit element of $\mathcal{G}_0$. Textbooks [4–6] tell us then that one can define a group structure $\mathcal{G}$ on the set $\mathcal{G}_0 \times \boldsymbol{Z}^\Lambda$ by taking z as an extension cocycle; *i.e.* one puts, for $g, g' \in \mathcal{G}_0$ and $f, f' \in \boldsymbol{Z}^\Lambda$,

$$(g, f)(g', f') := (gg', f + gf' + z_{g,g'})\,.$$

This is the desired group law, the cocycle condition guaranteeing associativity and $(e, 0)$ giving the unit element of $\mathcal{G}$. One checks that phase functions gauge–equivalent in Mermin's sense give the same cocycle (which also could be phrased cohomologically) and that all this extends the standard case, taken in Fourier space, where the functions involved specialize to linear functions on $\boldsymbol{R}^3$ restricted to Λ.

So far, however, our construction yields a group which is far too big, much bigger than the one constructed in [2]. This is because we haven't used the condition of $\boldsymbol{Z}$-linearity of the Φ_g when reduced mod $\boldsymbol{Z}$: what does it imply for the cocycles z? Being required to be integer-valued, $\boldsymbol{Z}$-linearity mod $\boldsymbol{Z}$ is automatic for them, but now our second point is that to z there is a cohomologous cocycle $\widetilde{z}$ that takes values in the abstract dual module Λ^* ($\boldsymbol{Z}$-linear maps $\Lambda \to \boldsymbol{Z}$). One therefore can consider the corresponding extensions $\mathcal{G}_0 \times \Lambda^*$ of $\mathcal{G}_0$ by Λ^* instead of $\boldsymbol{Z}^\Lambda$ which are considerably smaller and are equivalent to the construction in [2]. Note that $\mathcal{G}_0$ acts on Λ^* in the same way as on $\boldsymbol{Z}^\Lambda$.

In detail: cohomologous cocycles $z, \widetilde{z}$ on $\mathcal{G}_0$ with values in $\boldsymbol{Z}^\Lambda$ fulfill

$$\widetilde{z}_{g,g'} - z_{g,g'} = f_g - f_{gg'} + g f_{g'} \qquad \text{for some } f_g \in \boldsymbol{Z}^\Lambda\,;$$

they arise if Φ_g is replaced by $\widetilde{\Phi}_g = \Phi_g + f_g$. To make $\widetilde{z}$ Λ^*-valued, choose a basis $\{b_i\}$ for Λ and define $\widetilde{\Phi}_g$ by

$$\widetilde{\Phi}_g(\lambda) := \sum_i \lambda^i \Phi_g(b_i), \qquad \text{where } \lambda = \sum_i \lambda^i b_i\,.$$

Then $\widetilde{\Phi}_g - \Phi_g =: \widetilde{f}_g \in \boldsymbol{Z}^\Lambda$ by our assumption on Φ_g, and so, defining

$$\widetilde{z}_{g,g'} = \widetilde{\Phi}_g - \widetilde{\Phi}_{gg'} + g\widetilde{\Phi}_{g'}\,,$$

we have

$$\widetilde{z}_{g,g'} - z_{g,g'} = \widetilde{f}_g - \widetilde{f}_{gg'} + g\widetilde{f}_{g'}\,,$$

i.e. $\widetilde{z}$ and z are cohomologous cocycles. But now $\widetilde{z}_{g,g'}$ is $\boldsymbol{Z}$-valued *and* $\boldsymbol{Z}$-linear. The cocycle $\widetilde{z}$ thus takes values in Λ^* and defines ([5,6]) an element in $H^2(\mathcal{G}_0, \Lambda^*)$. This element is independent of the basis chosen for Λ. In

fact, if we start from another one, $\{\bar{b}_i\}$, and form $\bar{\tilde{z}}_{g,g'}$, correspondingly, the difference $\tilde{z}_{g,g'} - \bar{\tilde{z}}_{g,g'}$ is of the form $f_g - f_{gg'} + g f_{g'}$, where

$$f_g := \tilde{f}_g - \bar{\tilde{f}}_g = \tilde{\Phi}_g - \bar{\tilde{\Phi}}_g$$

is $\boldsymbol{Z}$-valued and $\boldsymbol{Z}$-linear, *i.e.* $f_g \in \Lambda^*$, thus $\tilde{z}$ and $\bar{\tilde{z}}$ are cohomologous as cocycles with values in Λ^*. Our new cocycle is again normalized if z was, so the group law of the extension $\mathcal{G}_0 \times \Lambda^*$ can be copied from above. As is well-known, up to isomorphism, the extension is uniquely determined by the cohomology class of $\tilde{z}$.

4. Concluding remark

In classical crystallography, one has the lattice $\mathcal{T}$ of translations in physical space and its reciprocal lattice Λ in Fourier space; the abstract dual of the latter as a $\boldsymbol{Z}$-module, Λ^*, can be identified with $\mathcal{T}$ again. In 'Copernican' quasicrystallography, one starts with a finitely generated free $\boldsymbol{Z}$-module Λ in Fourier space with more than three generators; its abstract dual Λ^* then has no interpretation as being embedded in physical space; but apart from this, the description of the space groups by elements of $H^2(\mathcal{G}_0, \Lambda^*)$ is the same. It is clear that this hardly scratches the surface of quasicrystallography, however.

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