match no. 9 pp. 15-20 1980

A mathematical note on Koptsik's definition of imperfect crystals

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In the following note I would like to give a formal mathematical definition of generalized wreath products and, then, to apply this concept towards the problem of how to define imperfect crystals and their symmetry groups,-both according to what I learned from Koptsik.

§ 1 Generalized wreath products.

Let G and H be groups with neutral elements 1_G and 1_H, such that G acts on H by automorphisms, i.e. there exists a map

(1) $$G \times H \longrightarrow H : (g,h) \longmapsto {}^g h$$

such that for $g, g_1, g_2 \in G$; $h_1, h_2, h \in H$

(2) $${}^g(h_1 h_2) = {}^g h_1 \cdot {}^g h_2, \quad {}^{(g_1 g_2)}h = {}^{g_1}\left({}^{g_2}h\right), \quad {}^{1_G}h = h.$$

Let A be a G-set, i.e. a set A together with a map

(3) $$G \times A \longrightarrow A : (g,a) \longmapsto ga ,$$

such that for $g_1, g_2 \in G$, $a \in A$

(4) $$(g_1 g_2)a = g_1(g_2 a) , \quad 1_G \cdot a = a.$$

Let B be a H-set on which G acts compatible with its action on H, i.e. a set B together with two maps

(5) $$H \times B \longrightarrow B : (h,b) \longmapsto h \cdot b; \; G \times B \longrightarrow B : (g,b) \longmapsto {}^g b$$

such that for $h_1, h_2, h \in H$; $g_1, g_2, g \in G$, $b \in B$

(6) $$(h_1 h_2) \cdot b = h_1 \cdot (h_2 \cdot b), \; 1_H \cdot b = b, \; {}^{(g_1 g_2)}b = {}^{g_1}\left({}^{g_2}b\right), \; {}^{1_G}b = b, \; {}^g(h \cdot b) = {}^g h \cdot {}^g b .$$

In this situation we want to define a generalized wreath product $H \int_A G = H^A \rtimes G$ of H and G with respect to A together with a natural action of this group on the cartesian product $A \times B$ and the function space B^A of all maps from A into B.

We do not exclude the case, in which G acts trivially on H and B, in which case our definitions reduce to that of ordinary wreath products.

At first we define the group H^A of all maps $f : A \longrightarrow H$ from A into H with multiplication defined as usual argument wise, i.e. - with $f_1, f_2 \in H^A$, $a \in A$ - by

(7) $$(f_1 \cdot f_2)\ (a) = f_1(a) \cdot f_2(a).$$

G acts on H^A in a natural way by automorphisms: for $g \in G$, $f \in H^A$ and $a \in A$

we put

$$(8)\qquad ({}^{g}f)\,(a) = {}^{g}f(g^{-1}a).$$

Then we have for $g_1, g_2, g \in G$; $f, f_1, f_2 \in H^A$

$$(9)\qquad {}^{g_1g_2}f = {}^{g_1}\left({}^{g_2}f\right),\quad {}^{1_G}f = f,\quad {}^{g}(f_1f_2) = {}^{g}f_1\cdot{}^{g}f_2$$

since for all $a \in A$:

$$(10)\qquad \left({}^{g_1}\left({}^{g_2}f\right)\right)(a) = {}^{g_1}\left(\left({}^{g_2}f\right)(g_1^{-1}a)\right) = {}^{g_1}\left({}^{g_2}f(g_2^{-1}g_1^{-1}a)\right)$$

$$= \left({}^{(g_1g_2)}f\right)(a),\quad \left({}^{1_G}f\right)(a) = f(a)$$

and

$$(11)\qquad \left({}^{g}f_1\cdot{}^{g}f_2\right)(a) = \left({}^{g}f_1\right)(a)\cdot\left({}^{g}f_2\right)(a) = {}^{g}f_1(g^{-1}a)\cdot{}^{g}f_2(g^{-1}a)$$

$$= {}^{g}\left(f_1(g^{-1}a)\cdot f_2(g^{-1}a)\right) = {}^{g}\left((f_1\cdot f_2)(g^{-1}a)\right) = \left({}^{g}(f_1\cdot f_2)\right)(a).$$

Thus we can define the semi-direct product $H^A \rtimes G$ of H^A and G, consisting of all pairs (f,g) with $f \in H^A$ and $g \in G$, and the multiplication, defined for $(f_1,g_1),(f_2,g_2) \in H^A \rtimes G$ by

$$(12)\qquad (f_1,g_1)\cdot(f_2,g_2) = (f_1\cdot{}^{g_1}f_2,\ g_1g_2).$$

We also write $H \int_A G$ instead of $H^A \rtimes G$.

The group H^A, identified with the set $H^A \times 1_G$ of pairs $(f,1_G)$, is normal in $H \int_A G$ and its factorgroup is canonically isomorphic to G. In H^A the group $(H^A)_{const}$ of all constant maps $A \longrightarrow H$, being identifiable with H, is G-invariant, (though not necessarily normal in H^A), thus $H \int_A G$ contains the semi-direct product $H \rtimes G$ in a canonical way as a subgroup. Further interesting G-invariant subgroups of H^A are for infinite A the subgroup $(H^A)_{fin}$ of all maps $f : A \longrightarrow H$ with $f(a) = 1_H$ for all but finitely many $a \in A$ and the group $(H^A)_{alm.const}$ of all almost constant maps $f : A \longrightarrow H$, i.e. all maps f, for which there exists $h \in H$ with $f(a) = h$ for all but finitely many $a \in A$. Obviously

$$(13)\qquad (H^A)_{alm.const.} = (H^A)_{fin.}\cdot(H^A)_{const} = (H^A)_{const}\cdot(H^A)_{fin}\ .$$

Moreover, if A possesses the structure of a topological space and each $g \in G$ acts continuously on A, the group $(H^A)_{disc}$ (or $(H^A)_{comp}$) of all maps $f : A \to H$ with $f(a) = 1_H$ for all $a \in A$ except for a in some discrete (or compact) subset $A' \subseteq A$, is a G-invariant subgroup of H^A, which will be of some importance later on.

Finally, for any G-invariant subgroup $H' \leq H$ the group H'^A of all maps $A \longrightarrow H'$ is a G-invariant subgroup of H^A and so are $(H'^A)_{const} = H'^A \cap (H^A)_{const}$,

$(H'^A)_{\text{alm.const}} = H'^A \cap (H^A)_{\text{alm.const.}}$ $(H'^A)_{\text{fin.}} = H'^A \cap (H^A)_{\text{fin}}$ and $(H'^A)_{\text{disc.}} = H'^A \cap (H^A)_{\text{disc.}}$

For all these G-invariant subgroups $V \leq H^A$ we can form the semi-direct product $V \rtimes G$ as a subgroup of $H \int_A G$. In particular, $H_1 \int_A G \leq H \int_A G$ for any G-invariant subgroup $H_1 \leq H$ of H.

Now let us define and study the action of $H \int_A G$ on $A \times B$ and on B^A. For $(f,g) \in H^A \rtimes G = H \int_A G$ and $(a,b) \in A \times B$ we put

(14) $$(f,g) \cdot (a,b) = (ga, f(ga) \cdot {}^{g}b).$$

Obviously $1_{H\int_A G} \cdot (a,b) = (a,b)$ and for $(f_1,g_1),(f_2,g_2) \in H \int_A G$

(15) $$\begin{aligned}(f_1,g_1)\Big((f_2,g_2)(a,b)\Big) &= (f_1,g_1)\Big(g_2a, f_2(g_2a) \cdot {}^{g_2}b\Big)\\ &= \Big(g_1g_2a, f_1(g_1g_2a) \cdot {}^{g_1}\Big(f_2(g_2a) \cdot {}^{g_2}b\Big)\Big) =\\ &= \Big(g_1g_2a, f_1(g_1g_2a) \cdot {}^{g_1}\Big(f_2(g_1^{-1} \cdot g_1g_2a)\Big) \cdot {}^{g_1g_2}b\Big) =\\ &= \Big(g_1g_2a, f_1(g_1g_2a) \cdot \Big({}^{g_1}f_2\Big)\Big(g_1g_2a\Big) \cdot {}^{g_1g_2}b\Big) =\\ &= \Big(f_1 \cdot {}^{g_1}f_2, g_1g_2\Big) \cdot (a,b) = \Big((f_1,g_1) \cdot (f_2,g_2)\Big)(a,b),\end{aligned}$$

so (14) defines indeed an action of $H \int_A G$ on $A \times B$. This implies an action of $H \int_A G$ on B^A, considered as a subset of $P(A \times B)$, the set of subsets of $A \times B$. More precisely, for $F : A \to B$ an element in B^A, $(f,g) \in H \int_A G$ and $a \in A$ we put

(16) $${}^{g}F : A \to B : a \mapsto {}^{g}(F(g^{-1}a)),$$

defining an action of G on B^A, and get

(17) $$\big((f,g)F\big)(a) = f(a) \cdot {}^{g}(F(g^{-1}a)) = f(a) \cdot ({}^{g}F)(a).$$

Our first result is

<u>Theorem 1:</u> If H acts transitively on B, then $H^A \leq H \int G$ acts transitively on B^A. If H acts fixed point free on B (i.e. if $h \cdot b = b$ for some $h \in H$ and some $b \in B$ implies $h = 1_H$), then $H^A \leq H \int_A G$ acts fixed point free on B^A.

<u>Proof:</u> If $F, F' \in B^A$ and H acts transitively on B, we may choose for $a \in A$ an element $f(a) \in H$ with $f(a) \cdot F(a) = F'(a)$ and thus $(f, 1_G) \cdot F = F'$.

If H acts fixed point free on B and $(f, 1_G) \cdot F = F$, then $f(a) \cdot F(a) = F(a)$ for all $a \in A$ implies $f(a) = 1_H$ for all $a \in A$ and thus $(f, 1_G) = 1_{H\int_A G}$.

<u>Corollary 1:</u> If H acts regularly on B (i.e. if H acts transitively and fixed point free on B), then H^A acts regularly on B^A.

For any $F \in B^A$ let $(H\int_A G)_F = \{(f,g) \in H\int_A G \mid (f,g) \cdot F = F\}$ be the (full) "symmetry group" of F. Since $(H\int_A G)_{(g,f)\cdot F} = (g,f) \cdot (H\int_A G)_F \cdot (g,f)^{-1}$, all symmetry groups are conjugate in $H\int_A G$, if H acts transitively on B. Thus, it seems more appropriate to classify elements $F, F', \ldots \in B^A$ with respect to the action of G, say, considered as a subgroup of $H\int_A G$, or some other significant subgroup.

Concerning the structure of $(H\int_A G)_F$, we have

Corollary 2: If H acts transitively/fixed point free/regularly on B and if $F \in B^A$, then the canonical map $H\int_A G \to G : (f,g) \mapsto g$ maps the symmetry group $(H\int_A G)_F$ of F surjectively/injectively/bijectively into G.

Proof: The kernel of $(H\int_A G)_F \to G : (f,g) \mapsto g$ consists of all $f \in H^A$ with $(f, 1_G) \cdot F = F$ and, thus, is trivial, if H acts fixed point free on B. If H acts transitively on B, we can find for each $g \in G$ some $f \in H^A$ with $(1_{H^A}, g) \cdot F = (f, 1_G) \cdot F$; so we have for any $g \in G$ some $f \in H^A$ with $(f^{-1}, g) \in (H\int_A G)_F$, and since this element $(f^{-1}, g) \in (H\int_A G)_F$ will be mapped onto g, we see, that the transitivity of the action of H on B implies surjectivity of $(H\int_A G)_F \to G$.

§ 2 Imperfect crystals

Now let A be the 3-dimensional euclidean space $\mathbb{E}^3$ and let G be the group $O(\mathbb{E}^3)$ of all isometries of $\mathbb{E}^3$. Thus $O(\mathbb{E}^3)$ contains the subgroup $O^+(\mathbb{E}^3)$ of index 2 of all proper (orientation preserving) isometries of $\mathbb{E}^3$ and the translational subgroup $T \leq O^+(\mathbb{E}^3)$, consisting of all translations of $\mathbb{E}^3$. Obviously $T \cong \mathbb{R}^3$, $O(\mathbb{E}^3)/T \cong O_3(\mathbb{R})$, the 3-dimensional orthogonal group, and $O(\mathbb{E}^3) \cong T \rtimes O_3(\mathbb{R}) = \mathbb{R}^3 \rtimes O(\mathbb{R}^3)$, the semi-direct product of $\mathbb{R}^3$ and $O(\mathbb{R}^3)$, taken with respect to the natural action of $O(\mathbb{R}^3)$ on $\mathbb{R}^3$. We write $\det(g) = +1$, if $g \in O^+(\mathbb{E}^3)$ and $\det g = -1$ otherwise.

For the choice of B and H we discuss several possibilities: we may either choose $B = B_o$ as just a finite set, consisting of various symbols $X_o, X_1, \ldots, X_n$ for chemical substances, particularly chemical elements, but including one symbol, say X_o, for the "empty substance", and $H = H_o$ as the group Σ_{B_o} of all permutations of B_o, with G acting trivially on B_o and H_o, or we may choose $B = B_1$ as a finite set, consisting of symbols $X_o, X_1, \ldots, X_k, X^+_{k+1}, X^-_{k+1}, \ldots, X^+_n, X^-_n$ for chemical substances, some of which (more precisely, the last n - k of which) come with a pregiven orientation + or - in our three-space, and we may choose $H = H_1$ to consist of all permutations π of $X_o, \ldots, X_k, X^+_{k+1}, X^-_{k+1}, \ldots, X^+_n, X^-_n$ which permute the $X_o, \ldots, X_k$ among themselves and the $X^+_{k+1}, X^-_{k+1}, \ldots, X^+_n, X^-_n$ in such a way, that $\pi(X^\varepsilon_i) = X^\eta_j \Leftrightarrow \pi(X^{-\varepsilon}_i) = X^{-\eta}_j$ $(i,j = k+1, \ldots, n;\ \varepsilon, \eta \in \{+,-\})$, with G acting trivially on H_1 and on $\{X_o,\dots,X_k\}$, but $gX_i^{\varepsilon} = X_i^{\varepsilon\cdot\det g}$ for $i = k+1,\dots,n$; $\varepsilon \in \{+,-\}$, $g \in G = O(\mathbb{E}^3)$.

Finally we may choose $B = B_2$ to consist of, say, $B_o \times S^2$ (or $B_1 \times S^2$ or $\{X_o,\dots,X_k\} \cup \{X_{k+1}^+, X_{k+1}^-,\dots,X_e^+,X_e^-\} \cup \{X_{e+1},\dots,X_n\} \times S^2$) with $S^2 \subseteq \mathbb{R}^3$ the unit sphere in $\mathbb{R}^3$, - so any element in B_2 consists - essentially - of a chemical substance X_i together with a pregiven direction in $\mathbb{E}^3$ -, and we may put $H_2 = H_o \times O(\mathbb{R}^3)$ (or $H_1 \times O(\mathbb{R}^3)$ or ...), acting on $B_o \times S^2$ component wise, with G acting on $H_2 = H_o \times O(\mathbb{R}^3)$ and $B = B_o \times S^2$ via the homomorphism $G = O(\mathbb{E}^3) \to O(\mathbb{R}^3)$ and the latter group's natural action on the second component, i.e. either by conjugation or the standard action of $O(\mathbb{R}^3)$ on S^2.

In any case we get a natural action of $H \int_{\mathbb{E}^3} O(\mathbb{E}^3)$ on $B^{\mathbb{E}_3}$. Now let $V \leq H^{\mathbb{E}^3}$ be G-invariant, e.g. one of the groups discussed above. The central definition of an imperfect crystal is now the following:

<u>Definition 1:</u> Using the above notations we define an element $F \in B^{\mathbb{E}^3}$ to be an imperfect crystal structure relative to $V \leq H^{\mathbb{E}^3}$, if the canonical map $H \int_{\mathbb{E}^3} G \to G$ maps $(V \rtimes G)_F$ onto a crystallographic subgroup U of G, i.e. a discrete subgroup with a compact quotient space.

To define equivalence of such imperfect crystal structures we imbed $G = O(\mathbb{E}^3)$ into the group $G_1 = A(\mathbb{E}^3)$ of affine transformations of $\mathbb{E}^3$, which acts on all H's and B's in a natural and compatible way. Thus we can form $H \int_{\mathbb{E}^3} G_1$ and consider subgroups $W \leq H \int_{\mathbb{E}^3} G_1$ of this group, e.g. G_1 itself, identified with $1 \int_{\mathbb{E}^3} G_1$, or $V \rtimes G_1$ in case V is not only G-, but also G_1- invariant. With these notations we have

<u>Definition 2:</u> Two imperfect crystal structures $F_1, F_2 \in B^{\mathbb{E}_3}$ are W-equivalent, it there exists some element $w \in W$ with $w(V \rtimes G)_{F_1} w^{-1} = (V \rtimes G)_{F_2}$.

Let us discuss some special cases:

In case $V = \{1\}$, the trivial group, we get the usual perfect crystal structures.

In case $B = B_o = \{X_o, X_1, X_2\}$ and $V = (H'^{\mathbb{E}^3})_{const}$ with $H' \leq H_o = \Sigma_{B_o}$ the subgroup of order 2, consisting of the identity and the permutation, permuting X_1 and X_2 and fixing X_o, we get - essentially - the well known Shubnikov-groups.

In case $B = B_o = \{X_o, X_1,\dots,X_n\}$ and $V = H'^{\mathbb{E}^3}$ with $H' \leq H_o = \Sigma_{B_o}$ consisting of some (or all) permutations fixing X_o, we get, at least, those imperfect crystals, whose <u>underlying</u> geometric crystal structure is perfect, i.e. the crystal structure, we get by neglecting the difference between the various substances $X_1,\dots,X_n$ and taking into account only their position in three space.

In case $B = B_o = \{X_o,\dots,X_n\}$ and $V = (H_o^{\mathbb{E}^3})_{fin}$ or $V = (H_o^{\mathbb{E}^3})_{comp}$ we get those crystal structures which differ from being perfect only at a finite or a compact set of places, whereas in case $V = (H_o^{\mathbb{E}^3})_{disc}$ we may get crystal structures of the following kind: at first we define an underlying perfect crystal structure $F : \mathbb{E}^3 \rightarrow B_o$, such that for any $x_i \in B_o$ the preimage $F^{-1}(x_i)$ is either empty or non-discrete and then we disturb F a little by changing its values at a discrete set of places.

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