BRACES, GENERALIZATIONS AND APPLICATIONS TO THE YANG–BAXTER EQUATION

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ABSTRACT. Braces were introduced by Rump to study non-degenerate involutive set-theoretic solutions of the Yang–Baxter equation. We generalize Rump's braces to the non-commutative setting and use this new structure to study not necessarily involutive non-degenerate set-theoretical solutions of the Yang–Baxter equation. Based on results of Bachiller and Catino and Rizzo, we develop an algorithm to enumerate and construct classical and non-commutative braces of small size (up to isomorphism). This algorithm is used to produce a database of classical and non-commutative braces of small size. The paper contains several open problems, questions and conjectures.

Introduction

The Yang–Baxter equation first appeared in theoretical physics and statistical mechanics in the works of Yang [38] and Baxter [4, 5] and it has led to several interesting applications in quantum groups and Hopf algebras, knot theory, tensor categories and integrable systems, see for example [25], [35] and [28]. In [14], Drinfeld posed the problem of studying this equation from the set-theoretical perspective.

Recall that a set-theoretical solution of the Yang–Baxter equation is a pair (X, r), where X is a set and

$$r: X \times X \to X \times X, \quad r(x,y) = (\sigma_x(y), \tau_y(x)), \quad x, y \in X,$$

is a bijective map such that

$$(r \times id)(id \times r)(r \times id) = (id \times r)(r \times id)(id \times r).$$

Such $\frac{1}{2}$ map $\frac{1}{2}$ is usually called a braiding.

A solution (X, r) is said to be non-degenerate if the maps σ_x and τ_x are bijective for each $x \in X$, and (X, r) is said to be involutive if $r^2 = \mathrm{id}_{X \times X}$. The seminal works of Etingof, Schedler and Soloviev [15], and Gateva-Ivanova and Van den Bergh [24], discussed algebraic and geometrical interpretations and introduced several structures associated with the class of non-degenerate involutive solutions. Such solutions have been intensively studied, see for example [18, 19, 17], [21, 22, 23], [20], [31, 30], [11], [13], [10], [6], [36], and [26].

It was in studying involutive solutions that Rump introduced in [31] the brace structure. In [12], Cedó, Jespers and Okniński, defined a left brace as an abelian group (A, +) with another group structure with multiplication $(a, b) \mapsto ab$ such that the compatibility condition

$$a(b+c) + a = ab + ac$$

holds for all $a, b, c \in A$. This definition is equivalent to that of Rump.

Many of the problems related to involutive solutions can be restated in terms of braces. Two prominent examples are the following:

• Is every finite solvable group an involutive Yang–Baxter group? Recall that an involutive Yang–Baxter group is a group isomorphic to the group generated by the set $\{\sigma_x : x \in X\}$, where

$$r: X \times X \to X \times X, \quad r(x,y) = (\sigma_x(y), \tau_y(x)),$$

is a non-degenerate involutive solution of the Yang-Baxter equation. Recently Rump [33] and Bachiller [1] found a solvable finite group that is not an involutive Yang-Baxter group.

 Are there good methods to contruct all finite non-degenerate involutive solutions to the Yang-Baxter equation? Brute force seems not to be good enough. In [3], Bachiller, Cedó and Jespers, give a method to construct all finite solutions of a given size. For it to work, one needs the classification of left braces.

Non-involutive solutions were studied by Soloviev [34] and Lu, Yan and Zhu [27]. Such solutions have applications in knot theory, since they produce powerful knot and virtual knots invariants, see for example [29] and the references therein. The following question naturally arises: Is there an algebraic structure similar to the brace structure useful for studying non-involutive solutions? This paper introduces the notion of non-commutative brace and provides an affirmative answer to the above question. Following the definition of a left brace of Cedó, Jespers and Okniński, we extend braces to the non-commutative setting. Remarkably, this new structure provides the right algebraic framework to study involutive and non-involutive braidings and allows us to restate the main results of [34], [27] and [37].

As in the case of involutive solutions, the classification of finite non-commutative braces is one of the main steps needed for constructing finite solutions of the Yang–Baxter equation. One of the main results of this paper is an explicit classification of classical and non-commutative braces of small size. An algorithm to construct all non-isomorphic classical and non-commutative braces of a given size is described. This heavily depends on results of Bachiller [1] and Catino and Rizzo [9]. This algorithm was used to build a database of classical and non-commutative braces, a good source of examples that gives an explicit and direct way to approach some of the problems related to the Yang–Baxter equation. The database is available as a library for GAP [16] and Magma [8] immediately from the authors on request.

The paper is organized as follows. In Section 1 we extend braces to the non-commutative setting and state their main properties. We prove in Theorem 1.11 that non-commutative braces are equivalent to bijective 1-cocycles. Section 2 is devoted to a study of quotients of non-commutative braces. In Section 3 the connection between non-commutative braces and the Yang–Baxter equation is explored. In Theorem 3.1 we generalize a result of Rump and produce a canonical solution for each non-commutative brace. Some reconstruction theorems similar to those of Etingof, Schedler and Soloviev [15], Lu, Yan and Zhu [27] and Soloviev [34] are given at the end of this section. The method for constructing classical and non-commutative braces is given in Section 4. Section 5 discusses the algorithm that produces and enumerates classical and non-commutative left braces and some consequences. Problems, questions and conjectures are discussed in Section 6.

1. Noncommutative left braces

Braces were introduced by Rump in [31] to study involutive solutions of the Yang–Baxter equation. The following definition generalizes braces to the non-commutative setting.

Definition 1.1. A non-commutative left brace is a group A with an additional group structure given by $(a,b) \mapsto a \star b$ such that

$$(1.1) a \star (bc) = (a \star b)a^{-1}(a \star c).$$

holds for all $a, b, c \in A$, where a^{-1} denotes the inverse of a with respect to the group structure given by $(a, b) \mapsto ab$.

Of course Rump's left braces are examples of non-commutative braces. These are braces where the group (A, \cdot) is abelian.

Definition 1.2. A homomorphism between two non-commutative left braces A and B is a map $f: A \to B$ such that f(ab) = f(a)f(b) and $f(a \star b) = f(a) \star f(b)$ for all $a, b \in A$. The kernel of f is

$$\ker f = \{ a \in A : f(a) = 1 \},\$$

where 1 denotes the identity of the group (A, \cdot) with multiplication $a \cdot b = ab$ for all $a, b \in A$.

Example 1.3. Let (A, \cdot) be a group. Then A is a non-commutative left brace with $a \star b = ab$ for all $a, b \in A$. Similarly, $a \star b = ba$ defines a non-commutative left brace structure over A. These braces are isomorphic if and only if (A, \cdot) is abelian.

Example 1.4. Let A and B be groups and let $\alpha: A \to \operatorname{Aut}(B)$ be a group homomorphism. Then $A \times B$ has a non-commutative brace structure given by

$$(a,b)(a',b') = (aa',bb'),$$

 $(a,b) \star (a',b') = (aa',b\alpha_a(b')),$

where $a, a' \in A$ and $b, b' \in B$.

Example 1.5. Let A and B be groups and let $\alpha: A \to \operatorname{Aut}(B)$ be a group homomorphism. Assume that A is abelian. Then $A \times B$ has a non-commutative brace structure given by

$$(a,b)(a',b') = (aa',b\alpha_a(b')),$$

 $(a,b) \star (a',b') = (aa',bb'),$

where $a, a' \in A$ and $b, b' \in B$.

Example 1.6. This example is motivated by the paper of Weinstein and Xu on the Yang-Baxter equation, see [37]. Let A be a group and A_+ , A_- be subgroups of A such that A admits a unique factorization as $A = A_+A_-$. Thus each $a \in A$ can be written in a unique way as $a = a_+a_-$ for some $a_+ \in A_+$ and $a_- \in A_-$. The map

$$A_{+} \times A_{-} \to A, \quad (a_{+}, a_{-}) \mapsto a_{+}(a_{-})^{-1},$$

is bijective. Using this map we transport the group structure of the direct product $A_+ \times A_-$ into the set A. For $a = a_+ a_- \in A$ and $b = b_+ b_- \in A$ let

$$a \star b = a_+ b a_-$$
.

Then (A, \star) is a group. Furthermore, A is a non-commutative left brace.

Lemma 1.7. Let A be a non-commutative left brace. Then the following hold:

- (1) $1 = 1_{\star}$, where 1_{\star} denotes the unit of the group (A, \star) .
- (2) $a \star (b^{-1}c) = a(a \star b)^{-1}(a \star c)$ for all $a, b, c \in A$.
- (3) $a \star (bc^{-1}) = (a \star b)(a \star c)^{-1}a$ for all $a, b, c \in A$.

Proof. The first claim follows from (1.1) with $c = 1_{\star}$. To prove the second claim let d = bc. Then (1.1) becomes $a \star d = (a \star b)a^{-1}(a \star b^{-1}d)$ and the claim follows. The third claim is proved similarly.

Remark 1.8. Let A be a non-commutative left brace. For each $a \in A$ the map

$$\lambda_a \colon A \to A, \quad b \mapsto a^{-1}(a \star b),$$

is bijective with inverse $\lambda_a^{-1} \colon A \to A$, $b \mapsto \overline{a} \star (ac)$, where \overline{a} is the inverse of a with respect to \star . It follows that

$$a \star b = a\lambda_a(b), \quad ab = a \star \lambda_a^{-1}(b)$$

hold for all $a, b \in A$.

The following proposition extends results of Rump and Gateva-Ivanova into the non-commutative setting, see [17, Prop. 3.3].

Proposition 1.9. Let A be a set and assume that A has two operations such that (A, \cdot) and (A, \star) are groups. Assume that $\lambda \colon A \to \mathbb{S}_A$, $a \mapsto \lambda_a$, is given by $\lambda_a(b) = a^{-1}(a \star b)$. The following are equivalent:

- (1) A is a non-commutative brace.
- (2) $\lambda_{a\star b}(c) = \lambda_a \lambda_b(c)$ for all $a, b, c \in A$.
- (3) $\lambda_a(bc) = \lambda_a(b)\lambda_a(c)$ for all $a, b, c \in A$.

Proof. Let us first prove that $(1) \implies (2)$. Let $a, b, c \in A$. Since A is a brace and $a \star b^{-1} = a(a \star b)^{-1}a$ by Lemma 1.7,

$$\lambda_a \lambda_b(c) = a^{-1}(a \star \lambda_b(c)) = a^{-1}(a \star (b^{-1}(b \star c)))$$

= $a^{-1}(a \star b^{-1})a^{-1}(a \star b \star c) = (a \star b)^{-1}(a \star b \star c) = \lambda_{a \star b}(c).$

Now we prove (2) \implies (3). Since $ab = a \star \lambda_a^{-1}(b)$ for all $a, b \in A$,

$$\lambda_a(bc) = \lambda_a(b \star \lambda_b^{-1}(c)) = a^{-1}(a \star b \star \lambda_b^{-1}(c))$$

$$= a^{-1}(a \star b)(a \star b)^{-1}(a \star b \star \lambda_b^{-1}(c))$$

$$= \lambda_a(b)\lambda_{a \star b}\lambda_b^{-1}(c) = \lambda_a(b)\lambda_a\lambda_b\lambda_b^{-1}(c) = \lambda_a(b)\lambda_a(c).$$

Finally we prove that (3) \implies (1). Let $a, b, c \in A$. Then

$$a^{-1}(a \star (bc)) = \lambda_a(bc) = \lambda_a(b)\lambda_a(c) = a^{-1}(a \star b)a^{-1}(a \star c),$$

and hence $a \star (bc) = (a \star b)a^{-1}(a \star c)$.

Corollary 1.10. Let A be a non-commutative left brace and

$$\lambda \colon (A, \star) \to \operatorname{Aut}(A, \cdot), \quad a \mapsto \lambda_a(b) = a^{-1}(a \star b).$$

Then λ is a group homomorphism.

Proof. It follows immediately from Proposition 1.9.

Let A and G be groups and assume that $G \times A \to A$, $(g, a) \mapsto g \cdot a$, is a left action of G on A by automorphisms. A *bijective* 1-cocyle is a bijective map $\pi \colon G \to A$ such that

(1.2)
$$\pi(gh) = \pi(g)(g \cdot \pi(h))$$

for all $g, h \in G$.

Theorem 1.11. Over any group (A, \cdot) the following data are equivalent:

- (1) A group G and a bijective 1-cocycle $\pi: G \to A$.
- (2) A non-commutative left brace structure over A.

Proof. Consider on A a second group structure given by

$$a \star b = \pi(\pi^{-1}(a)\pi^{-1}(b))$$

for all $a, b \in A$. Since π is a 1-cocycle and G acts on A by automorphisms,

$$a \star (bc) = \pi(\pi^{-1}(a)\pi^{-1}(bc)) = a(\pi^{-1}(a) \cdot (bc))$$
$$= a((\pi^{-1}(a) \cdot b)(\pi^{-1}(a) \cdot c)) = (a \star b)a^{-1}(a \star c)$$

holds for all $a, b, c \in A$.

Conversely, assume that A is a non-commutative left brace. Set G = A with the multiplication $(a,b) \mapsto a \star b$ and $\pi = \mathrm{id}$. By Corollary 1.10, $a \mapsto \lambda_a$, is a group homomorphism and hence G acts on A by automorphisms. Then (1.2) holds and therefore $\pi \colon G \to A$ is a bijective 1-cocycle.

Remark 1.12. The construction of Theorem 1.11 is categorical.

2. Ideals and quotients

Definition 2.1. Let A be a non-commutative brace. A normal subgroup I of (A, *) is said to be an ideal of A if Ia = aI and $\lambda_a(I) \subseteq I$ for all $a \in A$.

Example 2.2. Let $f: A \to B$ be a brace homomorphism. Then $\ker f$ is an ideal of A since

$$f(\lambda_a(x)) = \lambda_{f(a)}(f(x)) = 1$$

for all $x \in \ker f$ and $a \in A$.

Lemma 2.3. Let A be a non-commutative brace and $I \subseteq A$ be an ideal. Then the following hold:

- (1) I is a normal subgroup of (A, \cdot) .
- (2) $a \star I = aI$ for all $a \in A$.
- (3) I and A/I are non-commutative braces.

Proof. Let $a, b \in I$. Then $a^{-1}b = \lambda_a(\overline{a} \star b) \in I$ and hence I is a subgroup of (A, \cdot) . Remark 1.8 implies

$$aI = a \star I = I \star a = Ia$$

for all $a \in A$. Thus I is a normal subgroup of (A, \cdot) and hence I and A/I are non-commutative braces.

Definition 2.4. Let A be a non-commutative brace. The socle of A is

$$Soc(A) = \{a \in A : a \star b = ab, \ b(b \star a) = (b \star a)b \ for \ all \ b \in A\}.$$

Lemma 2.5. Let A be a non-commutative brace. Then Soc(A) is an ideal of A contained in the center of (A, \cdot) .

Proof. Let us first prove that Soc(A) is a subgroup of (A, \star) . Clearly $1 \in Soc(A)$. Let $a, a' \in A$ and $b \in A$. Then $a \star a' \in Soc(A)$ since

$$(a \star a') \star b = a \star (a' \star b) = a \star (a'b) = a(a'b) = (aa')b = (a \star a')b.$$

Now since $\overline{a} = a^{-1} \in \text{Soc}(A)$ and $b = (aa^{-1}) \star b = a \star (a^{-1} \star b) = a(a^{-1} \star b)$, it follows that $\overline{a}b = a^{-1}b = a^{-1} \star b = \overline{a} \star b$. Hence Soc(A) is a subgroup of (A, \star) .

A direct calculation proves that

(2.1)
$$\lambda_b(a) = b \star a \star \overline{b} \quad \text{for all } a \in \text{Soc}(A) \text{ and } b \in A.$$

Then it follows that $Soc(A) = \{a \in A : a \star b = ab, \lambda_b(a) \star b = b \star a \text{ for all } b \in A\}$. Let $a \in Soc(A)$ and $b, c \in A$. Then

$$\lambda_c \lambda_b(a) = \lambda_{c \star b}(a) = (c \star b) \star a \star \overline{c \star c} = c \star \lambda_b(a) \star \overline{c},$$

$$\lambda_b(a) c = b^{-1}(b \star a) c = (b \star a) b^{-1} c = b \star (a(\overline{b} \star c)) = b \star a \star \overline{b} \star c = \lambda_b(a) \star c.$$

Hence $\lambda_b(\operatorname{Soc}(A)) \subset \operatorname{Soc}(A)$ for all $b \in A$ and $\operatorname{Soc}(A)$ is a normal subgroup of (A, \star) by (2.1).

Now we prove that Soc(A) is central in (A, \cdot) . Let $a \in Soc(A)$, $b \in A$ and $c = \overline{b}$. Since

$$c\star(ba)=(c\star b)c^{-1}(c\star a)=c^{-1}(c\star a)=(c\star a)c^{-1}=c\star(ab),$$

it follows that ba = ab.

3. Braces and the Yang-Baxter equation

We turn our attention to the connection between non-commutative left braces and set-theoretic solutions of the Yang–Baxter equation. The following theorem generalizes a result of Rump to the non-commutative setting, see [12, Lemma 2].

Theorem 3.1. Let A be a non-commutative left brace. Then

$$(3.1) r_A \colon A \times A \to A \times A, r_A(a,b) = (\lambda_a(b), \lambda_{\lambda_a(b)}^{-1}((a \star b)^{-1}a(a \star b)),$$

is a non-degenerate solution of the Yang-Baxter equation. Furthermore, r_A is involutive if and only if ab = ba for all $a, b \in A$.

Remark 3.2. Recall from [27] that a braiding operator over a group (A, \star) with multiplication $m: (a, b) \mapsto a \star b$ is a bijective map $r: A \times A \to A \times A$ such that

- (1) $r(a \star b, c) = (id \times m)r_{12}r_{23}(a, b, c)$ for all $a, b, c \in A$,
- (2) $r(a, b \star c) = (m \times id) r_{23} r_{12}(a, b, c)$ for all $a, b, c \in A$,
- (3) r(a,1) = (1,a) and r(1,a) = (a,1) for all $a \in A$, and
- (4) $mr(a,b) = a \star b$ for all $a,b \in A$.

Braiding operators are equivalent to 1-bijective cocycles by [27, Thm. 2], and bijective 1-cocycles are equivalent to non-commutative braces by Theorem 1.11. One can prove that (3.1) is the braiding operator corresponding to the non-commutative left brace A under this equivalence.

Proof of Theorem 3.1. Every braiding operator is a non-degenerate solution of the Yang-Baxter equation by [27, Cor. 3]. Thus it is enough to prove that r_A is a braiding operator on (A, \star) . Since $\lambda_a^{-1}(b) = \overline{a} \star (ab)$ for all $a, b \in A$,

$$\lambda_{\lambda_a(b)}^{-1}((a\star b)^{-1}a(a\star b))=\overline{\lambda_a(b)}\star(\lambda_a(b)(a\star b)^{-1}a(a\star b))=\overline{\lambda_a(b)}\star(a\star b)$$

holds for all $a, b \in A$. Thus $mr(a, b) = a \star b$ for all $a, b \in A$. Clearly r(a, 1) = (1, a) and r(1, a) = (a, 1) for all $a \in A$. Let $a, b, c \in A$. By Corollary 1.10 one obtains

$$(\mathrm{id} \times m)(r_{12}r_{23}(a,b,c) = (\mathrm{id} \times m)r_{12}(a,\lambda_b(c),\overline{\lambda_b(c)} \star b \star c)$$

$$= (\mathrm{id} \times m)(\lambda_a\lambda_b(c),\overline{\lambda_a\lambda_b(c)} \star a \star \lambda_b(c),\overline{\lambda_b(c)} \star b \star c)$$

$$= (\lambda_a\lambda_b(c),\overline{\lambda_a\lambda_b(c)} \star a \star b \star c)$$

$$= r(a \star b,c).$$

From Remark 1.8 one obtains that

$$\lambda_a(b \star c) = \lambda_a(b)\lambda_{a \star b}(c)$$

holds for all $a, b, c \in A$. From this formula one deduces that

$$\lambda_a(b) \star \lambda_{\overline{\lambda_a(b)} \star a \star b}(c) = \lambda_a(b) \star \lambda_{\lambda_a(b)}^{-1} \lambda_a \lambda_b(c) = \lambda_a(b) \lambda_{a \star b}(c) = \lambda_a(b \star c).$$

holds for all $a,b,c \in A$. Then $r(a,b\star c)=(m\times \mathrm{id})r_{23}r_{12}(a,b,c)$ holds for all $a,b,c\in A$.

Corollary 3.3. Let A be a non-commutative left brace and $X \subseteq A$ be a subset of A. Assume $b\lambda_a(x)b^{-1} \in X$ for all $x \in X$ and $a, b \in A$. Then $r_A|_{X \times X}$ is a non-degenerate solution of the braid equation.

Proof. Clearly $\lambda_a(x) \in X$ and $bxb^{-1} \in X$ for all $a, b \in A$ and $x \in X$. Then it follows that $\lambda_{\lambda_x(y)}^{-1}((x \star y)^{-1}x(x \star y)) \in X$ for all $x, y \in X$. Now Theorem 3.1 implies the claim.

Example 3.4. Let A and B be groups and $\alpha: A \to \operatorname{Aut}(B)$ be a group homomorphism. The non-commutative brace of Example 1.4 yields the following solution:

$$\begin{split} r\colon (A\times B)\times (A\times B) &\to (A\times B)\times (A\times B),\\ r((a_1,b_1)(a_2,b_2)) &= ((a_2,\alpha_{a_1}(b_2)),(a_2^{-1}a_1a_2,b_2^{-1}\alpha_{a_2^{-1}}(b_1\alpha_{a_1}(b_2)))). \end{split}$$

Example 3.5. Let A be an abelian group, B be a group and $\alpha: A \to \operatorname{Aut}(B)$ be a group homomorphism. The non-commutative brace of Example 1.5 yields the following solution:

$$\begin{split} r\colon (A\times B)\times (A\times B) &\to (A\times B)\times (A\times B),\\ r((a_1,b_1)(a_2,b_2)) &= ((a_2,\alpha_{a_1^{-1}}(b_2)),(a_1,\alpha_{a_1^{-1}}(b_2^{-1})b_1b_2)). \end{split}$$

Example 3.6. Let A be the non-commutative left brace constructed in Example 1.6. The solution of Theorem 3.1 is similar to the solution constructed by Weinstein and Xu in terms of factorizable Poisson groups [37, Thm. 9.2]. The latter is $\tau r_A \tau$, where r_A is the solution of Theorem 3.1 and $\tau(x,y) = (y,x)$ for all x,y.

Based on [27], for each non-commutative left brace A we relate the solution given by Theorem 3.1 to the so-called Venkov solution, i.e.

$$s(a,b) = (b, b^{-1}ab), \quad a, b \in A.$$

Proposition 3.7. Let A be a non-commutative left brace. For each $n \in \mathbb{N}$ the map T_n given by

$$T_n(a_1,\ldots,a_{n-1},a_n)=(a_1,\lambda_{a_1}(a_2),\lambda_{a_1\star a_2}(a_3),\ldots,\lambda_{a_1\star \cdots \star a_{n-1}}(a_n))$$

is invertible and satisfies

$$(3.2) T_n r_{i,i+1} = s_{i,i+1} T_n$$

for all $n \geq 2$ and $i \in \{1, ..., n-1\}$, where $r_{i,i+1}$ and $s_{i,i+1}$ denote the actions of \mathbb{B}_n on $A^n = A \times \cdots \times A$ (n-times) induced from r and s respectively.

Proof. A direct calculation shows that T_n is invertible with inverse

$$T_n^{-1}(a_1,\ldots,a_n)=(a_1,\lambda_{a_1}^{-1}(a_2),\lambda_{a_1a_2}^{-1}(a_3),\ldots,\lambda_{a_1\ldots a_{n-1}}^{-1}(a_n)).$$

To prove (3.2) we proceed by induction on n. The case n=2 follows from a direct calculation. So assume that the claim holds for n-1. Since $T_n r_{1,2} = s_{1,2} T_n$ is the same as $T_2 r = s T_2$, we need to prove (3.2) for all $i \in \{2, \ldots, n-1\}$. Write

$$T_n = U_n(\mathrm{id} \times T_{n-1}),$$

where

$$U_n(a_1,\ldots,a_{n-1},a_n)=(a_1,\lambda_{a_1}(a_2),\ldots,\lambda_{a_1}(a_{n-1}),\lambda_{a_1}(a_n)).$$

Since each λ_a is an automorphism of (A, \cdot) , it follows that $U_n s_{i,i+1} = s_{i,i+1} U_n$ for $i \geq 2$ and hence (3.2) holds for all $i \geq 2$.

Remark 3.8. Proposition 3.7 also follows from [26, Prop. 6.2]. The map T_n is the so-called *guitar map*, see for example [26, §6].

The universal construction of Lu, Yan and Zhu, given in [27, Thm. 9] can be restated in the language of non-commutative left braces. Recall that the *enveloping* group of a solution (X, r) is the group G(X, r) generated by the elements of X and the relations

$$x \star y = \sigma_x(y) \star \tau_y(x), \quad x, y \in X.$$

Let $\iota \colon X \to G(X,r)$ be the canonical map.

Theorem 3.9. Let X be a set, $r: X \times X \to X \times X$, $r(x,y) = (\sigma_x(y), \tau_y(x))$ be a non-degenerate solution of the Yang–Baxter equation. Then there exists a unique brace structure over G(X,r) such that its associated solution r_G satisfies

$$r_G(\iota \times \iota) = (\iota \times \iota)r.$$

Furthermore, if B is a brace and $f: X \to B$ is a map such that $(f \times f)r = r_B(f \times f)$, then there exists a unique group homomorphism $\phi: G(X,r) \to B$ such that $f = \phi \iota$ and $(\phi \times \phi)r_G = r_B(\phi \times \phi)$.

Proof. The claim follows from the universal construction of [27, Thm. 9] and the equivalence between braiding operators and non-commutative braces, see Remark 3.2.

The following is essentially [34, Thm. 2.6].

Corollary 3.10. Let (X,r) be a finite non-degenerate solution of the Yang–Baxter equation. Then $G(X,r)/\operatorname{Soc}(G(X,r))$ is a finite brace.

Proof. It follows from Theorem 3.9 and Lemma 2.5.

4. Constructing non-commutative braces

Let A be a group. The *holomorph* of A is the group $\operatorname{Hol}(A) = \operatorname{Aut}(A) \ltimes A$, where the product is given by

$$(f,a)(g,b) = (fg,af(b))$$

for all $a, b \in A$ and $f, g \in Aut(A)$. Any subgroup H of Hol(A) acts on A

$$(4.1) (f,x) \cdot a = \pi_2((f,x)(\mathrm{id},a)) = xf(a), \quad a, x \in A, f \in \mathrm{Aut}(A),$$

where $\pi_2 \colon \operatorname{Hol}(A) \to A$, $(f, a) \mapsto a$. In particular $\operatorname{Hol}(A)$ acts transitively on A and the stabilizer of any $a \in A$ is isomorphic to $\operatorname{Aut}(A)$.

Recall that a subgroup H of $\operatorname{Hol}(A)$ is regular if for each $a \in A$ there exists a unique $(f, x) \in H$ such that xf(a) = 1.

Lemma 4.1. Let A be a group and H be a regular subgroup of $\operatorname{Hol}(A)$. Then $\pi_2|_H: H \to A, (f, a) \mapsto a$, is bijective.

Proof. We first prove that $\pi_2|_H$ is injective. Let $(f,a),(g,b)\in H$ be such that $\pi_2(f,a)=\pi_2(g,b)$. Then a=b. Since H is a subgroup,

$$(f,a)^{-1} = (f^{-1}, f^{-1}(a^{-1})) \in H, \quad (g,a)^{-1} = (g^{-1}, g^{-1}(a^{-1})) \in H,$$

and hence f = g since $f^{-1}(a)f^{-1}(a^{-1}) = g^{-1}(a)g^{-1}(a^{-1}) = 1$ and H is a regular subgroup.

Now we prove that $\pi_2|_H$ is surjective. Let $a \in A$. The regularlity of H implies the existence of an automorphism $f \in \operatorname{Aut}(A)$ such that $(f, f(a^{-1})) \in H$. Then $(f^{-1}, a) \in H$ and the claim follows.

The following results date back to Bachiller [1] and Catino and Rizzo [9].

Theorem 4.2. Let A be non-commutative brace. Then $\{(\lambda_a, a) : a \in A\}$ is a regular subgroup of $\operatorname{Hol}(A, \cdot)$. Conversely, if (A, \cdot) is a group and H is a regular subgroup of $\operatorname{Hol}(A, \cdot)$, then A is a non-commutative brace with $(A, \star) \simeq H$, where

$$a \star b = a f(b)$$

and
$$(\pi_2|_H)^{-1}(a) = (f, a) \in H$$
.

Proof. Since λ is a group homomorphism, it follows that $\{(\lambda_a, a) : a \in A\}$ is a subgroup of $\operatorname{Hol}(A, \cdot)$. The regularlity follows since (A, \star) is a group and $a\lambda_a(b) = a \star b$ holds for all $a, b \in A$, see [1, Prop. 2.3(1)].

Assume now that H is a regular subgroup. By Lemma 4.1, $\pi_2|_H$ is bijective. Use the bijection $\pi_2|_H$ to transport the product of H into A:

$$a \star b = \pi_2|_H ((\pi_2|_H)^{-1}(a)(\pi_2|_H)^{-1}(b)) = af(b),$$

where $a, b \in A$ and $(\pi_2|_H)^{-1}(a) = (f, a) \in H$. Then (A, \star) is a group and A is a non-commutative brace since

$$a\star(bc)=af(bc)=af(b)f(c)=af(b)a^{-1}af(c)=(a\star b)a^{-1}(a\star c)$$

holds for all $a, b, c \in A$.

Proposition 4.3. Let A be a group. There exists a bijective correspondence between non-commutative brace structures over A and regular subgroups of Hol(A). Moreover, isomorphic non-commutative braces structures over A correspond to conjugate subgroups of Hol(A) by elements of Aut(A).

Proof. Assume that the group A has two brace structures given by $(a,b) \mapsto a \star b$ and $(a,b) \mapsto a \times b$ and that $\phi \in \text{Aut}(A,\cdot)$ satisfies $\phi(a \star b) = \phi(a) \times \phi(b)$ for all $a,b \in A$. We claim that $\{(\lambda_a,a): a \in A\}$ and $\{(\mu_a,a): a \in A\}$, where $\lambda_a(b) = a^{-1}(a \star b)$ and $\mu_a(b) = a^{-1}(a \times b)$, are conjugate by ϕ . Since

$$\phi \lambda_a \phi^{-1}(b) = \phi(a^{-1}(a \star \phi^{-1}(b))) = \phi(a)^{-1}(\phi(a) \times b) = \mu_{\phi(a)}(b),$$

one obtains that $\phi(\lambda_a, a)\phi^{-1} = (\mu_{\phi(a)}, \phi(a))$ and hence the claim follows.

Conversely, let H and K be regular subgroups of $\operatorname{Hol}(A)$ and assume that there exists $\phi \in \operatorname{Aut}(A, \cdot)$ such that $\phi^{-1}H\phi = K$. Let $(f, a) = (\pi_2|_H)^{-1}(a) \in H$, $(g, a) = (\pi_2|_K)^{-1}(a) \in K$ and write $a \star b = af(b)$ and $a \times b = ag(b)$. Since $\phi(f, a)\phi^{-1} = (\phi f \phi^{-1}, \phi(a)) \in K$, it follows that $(\pi_2|_K)^{-1}(\phi(a)) = (\phi f \phi^{-1}, \phi(a))$. Then, since $\phi \in \operatorname{Aut}(A, \cdot)$,

$$\phi(a) \times \phi(b) = \phi(a)(\phi f \phi^{-1})(\phi(b)) = \phi(a)\phi(f(b)) = \phi(af(b)) = \phi(a \star b)$$

and hence the braces corresponding to H and K are isomorphic.

5. Computational results

We first present the algorithm used to enumerate non-commutative left brace structures over a given group A. The algorithm uses Theorem 4.2.

Algorithm 5.1. Let A be a finite group. To construct all non-commutative left brace structures over A we proceed as follows:

- (1) Compute the holomorph Hol(A) of A.
- (2) Compute the list of regular subgroups of Hol(A) of order |A| up to conjugation by elements of Aut(A).
- (3) For each representative H of regular subgroups of Hol(A) construct the map $p: A \to H$ given by $a \mapsto (f, f(a)^{-1})$, where $(f, f(a)^{-1}) \in H$. The triple $(H, A, p: A \to H)$ yields a non-commutative left brace structure over A with multiplication given by $a \star b = p^{-1}(p(a)p(b))$ for all $a, b \in A$.

Remark 5.2. To enumerate all non-commutative left brace structures over A the third step of Algorithm 5.1 is not needed.

Remark 5.3. Recall that a left brace is an abelian group (A, +) with a multiplication $(a, b) \mapsto ab$ such that a(b + c) + a = ab + ac holds for all $a, b, c \in A$. Left braces with additive group isomorphic to a given group A can be constructed applying Algorithm 5.1 to the abelian group A. In the second step of Algorithm 5.1 it is enough to compute the list of regular solvable subgroups of Hol(A), since the multiplicative group of a left brace is solvable by [15, Prop. 2.5].

Algorithm 5.1 was implemented both in GAP and Magma with different performances and were run on a Intel(R) Core(TM) i5-4440 CPU @3.10GHz with 16gb of RAM, under Linux.

5.1. Noncommutative left braces. For $n \in \mathbb{N}$ let c(n) be the number of non-isomorphic non-commutative left braces of size n.

The number of non-commutative left braces of size $n \leq 16$ has been determined using Algorithm 5.1. Table 5.1 shows some values of c(n). The calculation took about twenty minutes.

Table 5.1. The number of non-isomorphic non-commutative left braces.

n	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
c(n)	1	1	1	4	1	6	1	47	4	6	1	38	1	6	1	16 1605

5.2. **Left braces.** For $n \in \mathbb{N}$ let b(n) be the number of non-isomorphic left braces of size n.

The number of left braces (up to isomorphism) of size $n \le 120$ has been determined using Algorithm 5.1. Table 5.3 shows some values of b(n) and Table 5.2 gives runtimes for our Magma implementation for some examples. The construction of left braces requires considerably more CPU time, see Table 5.4 for some examples.

Table 5.2. Some runtimes for enumerating left braces of size n.

n	CPU time	b(n)
16	1 hour	357
48	18 hours	1708
54	5 minutes	80
72	1 hour	489
80	17 hours	1985
100	15 secs	51
108	28 hours	494
112	12 hours	1671

Table 5.3. The number of non-isomorphic left braces.

n	1	2	3	4	5	6	7	8	9	10	11	12
b(n)	1	1	1	4	1	2	1	27	4	2	1	10
n	13	14	15	16	17	18	19	20	21	22	23	24
b(n)	1	2	1	357	1	8	1	11	2	2	1	96
n	25	26	27	28	29	30	31	32	33	34	35	36
b(n)	4	2	37	9	1	4	1	?	1	2	1	46
n	37	38	39	40	41	42	43	44	45	46	47	48
b(n)	1	2	2	106	1	6	1	9	4	2	1	1708
n	49	50	51	52	53	54	55	56	57	58	59	60
b(n)	4	8	1	11	1	80	2	91	2	2	1	28
n	61	62	63	64	65	66	67	68	69	70	71	72
b(n)	1	2	11	?	1	4	1	11	1	4	1	489
n	73	74	75	76	77	78	79	80	81	82	83	84
b(n)	1	2	5	9	1	6	1	1985	?	2	1	34
n	85	86	87	88	89	90	91	92	93	94	95	96
b(n)	1	2	1	90	1	16	1	9	2	2	1	?
n	97	98	99	100	101	102	103	104	105	106	107	108
b(n)	1	8	4	51	1	4	1	106	2	2	1	494
n	109	110	111	112	113	114	115	116	117	118	119	120
b(n)	1	6	2	1671	1	6	1	11	11	2	1	395

With current computational resources, we were not able to compute the number of non-isomorphic left braces of orders 32, 64, 81 and 96.

Table 5.4. Some runtimes for constructing left braces of size n.

n	CPU time	b(n)
16	3 hours	357
54	40 minutes	80
72	24 hours	489
112	$5 \mathrm{days}$	1671

5.3. Two-sided left braces (radical rings). Recall that a brace B is a two-sided brace if (a+b)c+c=ac+bc holds for all $a,b,c\in B$. Two-sided braces are in bijective correspondence with radical rings [31]. Recall that a non-zero radical ring is a ring R without identity such that for each $x\in R$ there is $y\in R$ such that x+y+xy=0. Assume that R is a radical ring. Then the circle operation,

$$a \circ b = ab + a + b$$
, $a, b \in R$,

makes $(R, +, \circ)$ into a two-sided brace. Conversely, if A is a two-sided brace, the operation a * b = ab - a - b, $a, b \in A$ makes (A, +, *), into a radical ring.

To test whether a left brace is a two-sided brace one has the following lemma of Gateva-Ivanova, see [17, Cor. 3.5].

Lemma 5.4 (Gateva-Ivanova). Let A be a left brace. Then A is a two-sided brace if and only if

$$bc\lambda_{abc}^{-1}(c) = c\lambda_{ac}^{-1}(\lambda_a(b)c)$$

for all $a, b, c \in A$.

For $n \in \mathbb{N}$ let t(n) be the number of non-isomorphic two-sided braces of size n. Using the database of left braces constructed with Algorithm 5.1 and Lemma 5.4 one computes t(n). Table 5.5 shows the value of t(n) for $n \leq 24$.

Table 5.5. The number of non-isomorphic two-sided braces.

n	1	2	3	4	5	6	7	8	9	10	11	12
t(n)	1	1	1	4 4	1	1	1	22	4	1	1	4
n	13	14	15	16	17	18	19	20	21	22	23	24
t(n)	1	1	1	16 221	1	4	1	4	1	1	1	22

6. Further questions

In this section we collect some questions and conjectures that appear naturally after inspecting Table 5.3.

6.1. **Left braces.** We first collect some problems and conjectures related to the number of left braces.

Problem 6.1. Compute b(32), b(64), b(81) and b(96).

Table 5.3 suggests the following conjectures.

Conjecture 6.2. Let p > 3 be a prime number. Then

$$b(4p) = \begin{cases} 11 & \text{if } m \equiv 1 \mod 4, \\ 9 & \text{if } m \equiv 3 \mod 4. \end{cases}$$

Conjecture 6.3. Let p > 3 be a prime. Then

$$b(9p) = \begin{cases} 14 & \text{if } p \equiv 1 \mod 9, \\ 4 & \text{if } p \equiv 2, 5 \mod 9, \\ 11 & \text{if } p \equiv 4, 7 \mod 9. \end{cases}$$

Conjecture 6.4. Let p, q be prime numbers such that p < q and $q \not\equiv 1 \mod p$. Then $b(p^2q) = 4$.

We have used [7] and computer calculations to show that Conjectures 6.2 and 6.3 are true up to p = 997. Conjecture 6.4 was verified for several pairs of primes p, q such that p < q < 100.

6.2. Quaternionic braces. We now consider an important family of braces. Recall that for $m \in \mathbb{N}$ the generalized quaternion group is the group

$$Q_{4m} = \langle a, b : a^m = b^2, a^{2m} = 1, b^{-1}ab = a^{-1} \rangle.$$

Definition 6.5. A brace is a quaternion brace if its multiplicative group is isomorphic to some quaternion group.

Conjecture 6.6. For $m \in \mathbb{N}$ let q(4m) be the number of isomorphism classes of quaternion braces of size 4m. Then for m > 2

$$q(4m) = \begin{cases} 2 & \text{if } m \text{ is odd,} \\ 7 & \text{if } m \equiv 0 \bmod 8, \\ 9 & \text{if } m \equiv 4 \bmod 8, \\ 6 & \text{if } m \equiv 2 \bmod 8 \text{ or } m \equiv 6 \bmod 8. \end{cases}$$

We have checked Conjecture 6.6 for all $m \leq 512$. It seems natural to ask the following questions.

Question 6.7. Which finite abelian groups appear as the additive group of a quaternion brace?

For $m \in \{2, ..., 512\}$ the additive group of a quaternion brace of size m is isomorphic to one of the following groups:

$$\mathbb{Z}_{4m}, \mathbb{Z}_{2m} \times \mathbb{Z}_2, \mathbb{Z}_m \times \mathbb{Z}_2 \times \mathbb{Z}_2, \mathbb{Z}_m \times \mathbb{Z}_4, \mathbb{Z}_{m/2} \times \mathbb{Z}_2 \times \mathbb{Z}_2 \times \mathbb{Z}_2.$$

By inspection, one sees that the groups $\mathbb{Z}_m \times \mathbb{Z}_2^2$ appear whenever $m \equiv 2, 4, 6 \mod 8$ and the groups $\mathbb{Z}_m \times \mathbb{Z}_4$ and $\mathbb{Z}_{m/2} \times \mathbb{Z}_2^3$ appear whenever $m \equiv 4 \mod 8$.

Question 6.8. For m > 2 let A be a finite abelian group size 4m. Compute the number of isomorphism classes of quaternion braces of size 4m with additive group isomorphic to A.

In $[3, \S 5]$ quaternion braces of size 2^k are mentioned as an important class of braces which could be useful to classify a certain family of involutive non-degenerate solutions of the Yang–Baxter equation. Conjecture 6.6 implies the following:

Conjecture 6.9. There are seven classes of isomorphism of quaternion braces of size 2^k for k > 4.

Conjecture 6.9 was verified for all $k \in \{5, 6, 7, 8, 9\}$. Table 6.1 sums up our findings related to this important subclass of braces.

TABLE 6.1. Number of braces with multiplicative group isomorphic to the quaternion group Q_{2^k} with k > 4.

Additive Group	Number of Braces					
\mathbb{Z}_{2^k}	1					
$\mathbb{Z}_{2^{k-1}} \times \mathbb{Z}_2$	6					

Remark 6.10. The classification of left braces over cyclic groups was done by Rump in [32]. Recently, in [2], Bachiller classified left braces of size p^2 and p^3 , where p is a prime number. The techniques used in these papers might prove useful to address the questions, problems and conjectures in this section.

Acknowledgement. This work is partially supported by CONICET, FONCyT PICT-2014-1376 and ICTP. We thank Leandro del Pezzo for the computer where some calculations were performed, David Bachiller for his suggestions, and Victoria Lebed for several useful comments and corrections.

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