



# Reachability problems in quaternion matrix and rotation semigroups

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## ABSTRACT

We examine computational problems on quaternion matrix and rotation semigroups. It is shown that in the ultimate case of quaternion matrices, in which multiplication is still associative, most of the decision problems for matrix semigroups are undecidable in dimension two. The geometric interpretation of matrix problems over quaternions is presented in terms of rotation problems for the 2- and 3-sphere. In particular, we show that the reachability of the rotation problem is undecidable on the 3-sphere and other rotation problems can be formulated as matrix problems over complex and hypercomplex numbers.

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## 1. Introduction

Quaternions have long been used in many fields including computer graphics, robotics, global navigation and quantum physics as a useful mathematical tool for formulating the composition of arbitrary spatial rotations and establishing the correctness of algorithms founded upon such compositions.

Many natural questions about quaternions are quite difficult and correspond to fundamental theoretical problems in mathematics, physics and computational theory. Unit quaternions actually form a *double cover* of the rotation group  $SO_3$ , meaning each element of  $SO_3$  corresponds to two unit quaternions. This makes them expedient for studying rotation and angular momentum and they are particularly useful in quantum mechanics. The group of unit quaternions form the group  $SU_2$  which is the special unitary group. The large number of applications has renewed interest in quaternions and quaternion matrices [1,10,17,20,21].

The multiplication of quaternions is not commutative and this leads to many problems with their analysis. In particular, defining the determinant and finding the eigenvalues and the inverse of a quaternion matrix are unexpectedly difficult problems [21]. In this paper, we study decision questions about semigroups of quaternions, quaternion matrices and rotations, such as reachability questions, membership problems, freeness problems, etc. More research on these problems for matrix semigroups over  $\mathbb{Z}, \mathbb{Q}, \mathbb{C}$  can be found in [3–6,8,9,11,12,16]. There are two major points of this work that we would like to highlight.

First, we investigated classical matrix decision problems for low-dimensional quaternion matrices. The results for matrices over  $\mathbb{Z}, \mathbb{Q}, \mathbb{C}$  are not easily transferable to the case of quaternions and thus there are no results on *computational problems* for quaternions and quaternion matrices. Most of the problems for  $2 \times 2$  matrices were open for any number field. In this paper, we show that all standard reachability problems are undecidable for  $2 \times 2$  quaternion matrix semigroups. Moreover, our construction uses unitary quaternions that have a special interest in terms of rotations. After the quaternions, the hypercomplex numbers lose the associativity property and thus no longer form a semigroup. Due to this fact we think that

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our current research on quaternion matrices gives a more complete picture of decision problems for matrix semigroups. Then we study these problems for a case of Lipschitz integers and state several open problems.

The second important point of the paper is establishing connections between classical matrix semigroup problems and reachability problems for semigroups of rotations. In fact, using unit quaternions for encoding computational problems gives us an opportunity to formulate and prove several interesting results in terms of three- and four-dimensional rotations defined by quaternions. In particular, we show that the point-to-point rotation problem for the 3-sphere is undecidable. The same problem for the 2-sphere is open and can be formulated as a special case of the scalar reachability problem for matrix semigroups that we show is undecidable in general. As an additional benefit, the results on rotation semigroups give immediate corollaries for a class of orthogonal matrix semigroups.

The paper is organized as follows. In the second section, we give all definitions about quaternions and their matrix representation and a mapping between words and quaternions that will be used in our proofs. The third section contains the main results of the paper on undecidable problems (freeness, membership and reachability) in quaternion matrix semigroups. We prove that the membership problem for  $2 \times 2$  rational quaternion matrix semigroups is undecidable. We use a novel technique of PCP encoding, allowing us to encode pairs of words by separate matrices and force them to appear in the right order for a specific product. Then we show that the problem of deciding if any diagonal matrix is in a quaternion matrix semigroup, that has its own interest in a context of control theory, is undecidable. Then we study these problems for the case of Lipschitz integers. In the last section, the geometric interpretation of matrix problems over quaternions is presented in terms of rotation problems for the 2- and 3-sphere.

## 2. Preliminaries

We use the standard denotations  $\mathbb{N}, \mathbb{Z}^+, \mathbb{Q}$  to denote the natural numbers, positive integers and rational numbers, respectively.

In a similar style to complex numbers, rational quaternions, which are hypercomplex numbers, can be written  $\vartheta = a + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$  where  $a, b, c, d \in \mathbb{Q}$ . To ease notation let us define the vector:  $\mu = (1, \mathbf{i}, \mathbf{j}, \mathbf{k})$  and it is now clear that  $\vartheta = (a, b, c, d) \cdot \mu$  where  $\cdot$  denotes the inner or ‘dot’ product. We denote rational quaternions by  $\mathbb{H}(\mathbb{Q})_0$ . Quaternions with real part 0 are called *pure quaternions* and denoted by  $\mathbb{H}(\mathbb{Q})_0$ .

Quaternion addition is simply the componentwise addition of elements.

$$(a_1, b_1, c_1, d_1)\mu + (a_2, b_2, c_2, d_2)\mu = (a_1 + a_2, b_1 + b_2, c_1 + c_2, d_1 + d_2)\mu.$$

It is well known that quaternion multiplication is not commutative. Multiplication is completely defined by the equations  $\mathbf{i}^2 = \mathbf{j}^2 = \mathbf{k}^2 = -1$ ,  $\mathbf{ij} = \mathbf{k}$ ,  $\mathbf{jk} = \mathbf{i}$ ,  $\mathbf{ki} = \mathbf{j}$  and  $\mathbf{ji} = -\mathbf{k}$ ,  $\mathbf{ik} = -\mathbf{j}$ ,  $\mathbf{kj} = -\mathbf{i}$ . Thus for two quaternions  $\vartheta_1 = (a_1, b_1, c_1, d_1)\mu$  and  $\vartheta_2 = (a_2, b_2, c_2, d_2)\mu$ , we can define their product as

$$\begin{aligned} \vartheta_1 \vartheta_2 = & (a_1 a_2 - b_1 b_2 - c_1 c_2 - d_1 d_2) + (a_1 b_2 + b_1 a_2 + c_1 d_2 - d_1 c_2)\mathbf{i} \\ & + (a_1 c_2 - b_1 d_2 + c_1 a_2 + d_1 b_2)\mathbf{j} + (a_1 d_2 + b_1 c_2 - c_1 b_2 + d_1 a_2)\mathbf{k}. \end{aligned}$$

In a similar way to complex numbers, we define the conjugate of  $\vartheta = (a, b, c, d) \cdot \mu$  by  $\bar{\vartheta} = (a, -b, -c, -d) \cdot \mu$ . We can now define a norm on the quaternions by  $\|\vartheta\| = \sqrt{\vartheta \bar{\vartheta}} = \sqrt{a^2 + b^2 + c^2 + d^2}$ . Any non-zero quaternion has a multiplicative (and obviously an additive) inverse [13]. Note also that  $\vartheta_1 = (1, 0, 0, 0)\mu \in \mathbb{H}$  is the multiplicative identity quaternion which is clear from the multiplication shown above. The other properties of being a division ring can be easily checked.

A *unit* quaternion has norm 1 and corresponds to a rotation in the three-dimensional space. Given a unit vector  $\vec{r} = (r_1, r_2, r_3)$  and a rotation angle  $0 \leq \theta < 2\pi$ , we would like to find a quaternion transformation to represent a rotation of  $\theta$  radians of a point  $P' = (x, y, z) \in \mathbb{Q}^3$  about the  $\vec{r}$  axis. To facilitate this, we require an encoding of  $P'$  as a pure quaternion  $P$ , namely  $P = (0, x, y, z) \cdot \mu \in \mathbb{H}(\mathbb{Q})_0$ .

Let us define a function  $\psi_q : \mathbb{H}(\mathbb{Q}) \mapsto \mathbb{H}(\mathbb{Q})$  by  $\psi_q(P) = qPq^{-1}$  where  $q, P \in \mathbb{H}(\mathbb{Q})$  and  $\|q\| = 1$ . If  $q$  is correctly chosen to represent a rotation of  $\theta$  about a unit axis  $r$ , then this function will return a pure quaternion of the form  $(0, x', y', z') \cdot \mu$  where  $(x', y', z') \in \mathbb{Q}^3$  is the correctly rotated point.

It is well known (see, for example, [13]) that:  $\vartheta = (\cos \frac{\theta}{2}, \vec{r} \sin \frac{\theta}{2}) \cdot \mu$  represents a rotation of angle  $\theta$  about the  $\vec{r}$  axis. Therefore using  $\psi_\vartheta(P)$  as just described rotates  $P$  as required. This will be used in the next section.

All possible unit quaternions correspond to points on the 3-sphere. Any pair of unit quaternions  $p, q$  represent a four-dimensional rotation. Given a point  $x \in \mathbb{H}(\mathbb{Q})$ , we define a rotation of  $x$ , by  $px\bar{q}$  [19]. Also we use the notation  $SU_2$  to denote the special unitary group, the double cover of the rotation group  $SO_3$ .

The length of quaternions is multiplicative and the semigroup of Lipschitz integers with multiplication is closed. The fact that  $\|q_1 q_2\| = \|q_1\| \cdot \|q_2\|$  follows since the determinant of the matrix representation of a quaternion we define in Section 2.2 corresponds to the modulus and is multiplicative. This result will be required later.

### 2.1. Word morphisms

Let  $\Sigma = \{a, b\}$  be a binary alphabet,  $\vec{u} = (1, 0, 0)$  and  $\vec{v} = (0, 1, 0)$ . We define the homomorphism  $\varphi : \Sigma^* \times \mathbb{Q} \mapsto \mathbb{H}(\mathbb{Q})$  by:

$$\varphi(a,\theta) = \left( \cos\left(\frac{\theta}{2}\right), \vec{u} \sin\left(\frac{\theta}{2}\right) \right) \cdot \mu \text{ and } \varphi(b,\theta) = \left( \cos\left(\frac{\theta}{2}\right), \vec{v} \sin\left(\frac{\theta}{2}\right) \right) \cdot \mu,$$

where  $\theta \in \mathbb{Q} \in [0, 2\pi)$ , i.e.  $\varphi(a,\theta)$  is a rotation of angle  $\theta$  about the  $\vec{u}$  axis and  $\varphi(b,\theta)$  is a rotation of angle  $\theta$  about the  $\vec{v}$  axis.  $\varphi(\varepsilon,\theta) = \vartheta_I$  is the multiplicative identity element of the division ring of rational quaternions. Note that  $\vec{u} \cdot \vec{v} = 0$  and  $\|\vec{u}\| = \|\vec{v}\| = 1$ , thus these two vectors are orthonormal.

Let us define a specific instance of this morphism. Let  $\alpha = 2 \arccos\left(\frac{3}{5}\right) \in \mathbb{R}$ . Now we define  $\gamma : \Sigma^* \mapsto \mathbb{H}(\mathbb{Q})$  where  $\gamma(a) = \varphi(a,\alpha)$ ,  $\gamma(b) = \varphi(b,\alpha)$  and  $\gamma(\varepsilon) = (1,0,0,0)\mu = \vartheta_I$ . This gives the homomorphism:

$$\gamma(a) = \left( \cos\left(\arccos\left(\frac{3}{5}\right)\right), \vec{u} \sin\left(\arccos\left(\frac{3}{5}\right)\right) \right) \cdot \mu = \left( \frac{3}{5}, \frac{4}{5}, 0, 0 \right) \cdot \mu \tag{1}$$

$$\gamma(b) = \left( \cos\left(\arccos\left(\frac{3}{5}\right)\right), \vec{v} \sin\left(\arccos\left(\frac{3}{5}\right)\right) \right) \cdot \mu = \left( \frac{3}{5}, 0, \frac{4}{5}, 0 \right) \cdot \mu \tag{2}$$

which follows from the identity  $\cos^2\theta + \sin^2\theta = 1$  since  $\sqrt{1 - \left(\frac{3}{5}\right)^2} = \frac{4}{5}$ .

We can see that the quaternions in the image of  $\gamma$  are of unit length, i.e.  $\forall w \in \Sigma^*, \|\gamma(w)\| = 1$  since quaternion length is multiplicative ( $\|q_1q_2\| = \|q_1\| \cdot \|q_2\|$ , which we proved in Section 2) and  $\gamma(a), \gamma(b)$  have unit length.

**Lemma 1.** *The mapping  $\gamma : \Sigma^* \mapsto \mathbb{H}(\mathbb{Q})$  is a monomorphism.*

**Proof.** It was proven in [18] that if  $\cos(\theta) \in \mathbb{Q}$  then the subgroup of  $SO_3(\mathbb{R})$  generated by rotations of angle  $\theta$  about two perpendicular axes is free iff  $\cos(\theta) \neq 0, \pm \frac{1}{2}, \pm 1$ . We note that in the definition of  $\gamma$  we use a rotation about two orthonormal axes  $\vec{u}, \vec{v}$ . We use a rotation of  $\alpha = 2 \arccos\frac{3}{5}$ . From basic trigonometry,  $\cos(2 \arccos(\frac{3}{5})) = -\frac{7}{25}$  and  $\sin(2 \arccos(\frac{3}{5})) = \frac{24}{25}$  thus the cosine and sine of both angles are rational and not equal to  $0, \pm \frac{1}{2}, \pm 1$  (we only require this of the cosine) as required. We showed that all elements of the quaternions are rational, thus we have a free subgroup of  $SO_3(\mathbb{Q})$  generated by  $\gamma(a), \gamma(b) \in \mathbb{H}(\mathbb{Q})$ . Note that the conditions mentioned are guaranteed to give a free group but are not necessary for freeness, see [10].  $\square$

**Post’s correspondence problem (PCP)**—Given two (finite) alphabets  $\Gamma, \Sigma$  and two morphisms  $h, g : \Gamma^* \mapsto \Sigma^*$ , it is undecidable in general whether there exists a solution  $w \in \Gamma^+$  such that  $h(w) = g(w)$ . We can assume without loss of generality that  $\Sigma$  is binary by using a straightforward encoding. It was shown that the problem is undecidable when the instance size  $|\Gamma| \geq 7$  in [15]. We denote by  $n_p$  the smallest instance size for which PCP is undecidable (thus,  $n_p \leq 7$ ).

### 2.2. Matrix representations

It is possible to represent a quaternion  $\mathbb{H}(\mathbb{Q})$  by a matrix  $M \in \mathbb{C}^{2 \times 2}$ . For a general quaternion  $\vartheta = (a,b,c,d) \cdot \mu$  we define the matrix:

$$M = \begin{pmatrix} a + b\mathbf{i} & c + d\mathbf{i} \\ -c + d\mathbf{i} & a - b\mathbf{i} \end{pmatrix}.$$

**Corollary 2.** *There is a class of  $2 \times 2$  complex unitary matrices forming a free group.*

**Proof.** We can define a morphism similar to  $\gamma$  which instead maps to two-dimensional complex matrices:

$$\zeta(a) = \begin{pmatrix} \frac{3}{5} + \frac{4}{5}\mathbf{i} & 0 \\ 0 & \frac{3}{5} - \frac{4}{5}\mathbf{i} \end{pmatrix}, \quad \zeta(b) = \begin{pmatrix} \frac{3}{5} & \frac{4}{5} \\ -\frac{4}{5} & \frac{3}{5} \end{pmatrix}, \quad \zeta(\varepsilon) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Note that these matrices are unitary, therefore let  $\zeta(a^{-1}) = \zeta(a)^{-1} = \zeta(a)^*$  and  $\zeta(b^{-1}) = \zeta(b)^{-1} = \zeta(b)^*$  where  $*$  denotes the Hermitian transpose.

Thus we have an injective morphism  $\zeta : (\Sigma \cup \bar{\Sigma})^* \mapsto \mathbb{C}^{2 \times 2}$ . Since  $\gamma$  forms a free group of quaternions,  $\zeta$  forms a free group over  $\mathbb{C}^{2 \times 2}$ .  $\square$

Also note that we can define such matrices for any two orthonormal vectors where the rotation angle  $\theta$  satisfies  $\cos(\theta) \in \mathbb{Q}$  and  $\cos(\theta) \neq 0, \pm \frac{1}{2}, \pm 1$ .

### 3. Quaternion matrix semigroups

We will now show an undecidability result, a variant of which was considered by A. Markov where he showed undecidability for two sets of unimodular  $2 \times 2$  integral matrices, see [14,11].

**Theorem 3.** Given two sets  $A = \{a_1, a_2, \dots, a_n\}$  and  $B = \{b_1, b_2, \dots, b_n\}$ , where  $A, B \subset \mathbb{H}(\mathbb{Q})$ , it is undecidable whether there exists a non-empty sequence of indices  $(r_1, r_2, \dots, r_m)$  such that  $a_{r_1} a_{r_2} \dots a_{r_m} = b_{r_1} b_{r_2} \dots b_{r_m}$ , this holds for  $n = n_p$ .

**Proof.** We use a reduction of Post’s correspondence problem and the morphism  $\gamma$  defined in Section 2. Given two alphabets  $\Gamma, \Sigma$ , such that  $\Sigma$  is binary, and an instance of the PCP,  $(h, g) : \Gamma^* \mapsto \Sigma^*$ . We proved in Lemma 1 that  $\gamma$  is a monomorphism between  $\Sigma^*$  and  $\mathbb{H}(\mathbb{Q})$ . Thus let us define a new pair of morphisms  $(\rho, \tau)$  to map  $\Gamma^+ \times \Gamma^+$  directly into  $\mathbb{H}(\mathbb{Q}) \times \mathbb{H}(\mathbb{Q})$  (we can think of this as  $SU_2 \times SU_2$  since each of these unit quaternions represents an element of  $S^3$  (the 3-sphere)). For any  $w \in \Gamma^+$ , let  $\rho(w) = \gamma(h(w))$  and  $\tau(w) = \gamma(g(w))$ .

Thus for an instance of PCP,  $\Gamma = \{a_1, a_2, \dots, a_m\}$ ,  $(h, g)$ , we instead use the pair of morphisms  $(\rho, \tau)$ . Define two semigroups  $S_1, S_2$  which are generated, respectively, by  $\{\rho(a_1), \rho(a_2), \dots, \rho(a_m)\}$  and  $\{\tau(a_1), \tau(a_2), \dots, \tau(a_m)\}$ . We see their exists a solution to the given instance of PCP iff  $\exists w \in \Gamma^+$  such that  $\rho(w) = \tau(w)$ .  $\square$

We now move to an extension of the Theorem 3 where it is no longer necessary to consider the index sequence. Markov obtained a similar result by extending the dimension of the integral matrices to  $4 \times 4$  [14]. See also [3,11], where the authors improve Markov’s results to  $3 \times 3$  integral matrices.

**Theorem 4.** Given two semigroups  $S, T$ , generated by  $A, B$ , respectively, such that  $A = \{A_1, A_2, \dots, A_n\}$  and  $B = \{B_1, B_2\}$  where  $A, B \subset \mathbb{H}(\mathbb{Q})^{2 \times 2}$ , it is undecidable if  $S \cap T = \emptyset$ . Furthermore, all matrices in  $A, B$  can be taken to be diagonal.

**Proof.** Given an instance of PCP,  $(h, g)$  where  $h, g : \Gamma^* \mapsto \Sigma^*$ . We use the monomorphisms  $\rho, \tau : \Gamma^* \mapsto \mathbb{H}(\mathbb{Q})$  introduced in Theorem 3. For each  $a \in \Gamma$  we define:

$$A_a = \begin{pmatrix} \rho(a) & 0 \\ 0 & \tau(a) \end{pmatrix}$$

and these matrices form the generator for the semigroup  $S$ . For the second semigroup,  $T$ , we simply wish to encode each symbol from  $\Sigma$  in the [1,1] and [2,2] elements using the morphism  $\gamma : \Sigma^* \mapsto \mathbb{H}(\mathbb{Q})$  which was shown to be injective in Lemma 1:

$$B_1 = \begin{pmatrix} \gamma(a) & 0 \\ 0 & \gamma(a) \end{pmatrix}, \quad B_2 = \begin{pmatrix} \gamma(b) & 0 \\ 0 & \gamma(b) \end{pmatrix}.$$

We see that there exists  $M \in S$  such that  $M_{[1,1]} = M_{[2,2]}$  iff there exists a solution  $w \in \Gamma^+$  to the instance of the PCP. This follows since element [1,1] of  $M$  encodes  $h(w)$  and element [2,2] encodes  $g(w)$ . Clearly any such matrix  $M$  is also in  $T$  since every matrix in  $T$  corresponds to an encoding of all words over  $\Sigma^+$  in the top left and bottom right elements. Note that all matrices are diagonal and unitary.  $\square$

The previous two theorems used two separate semigroups. It is more natural to ask whether a particular element is contained within a *single* semigroup. For example, the mortality problem asks if the zero matrix is contained in an integral matrix semigroup and was shown to be undecidable in dimension 3 (see [16]). We showed that in dimension 4 the membership for any  $k$ -scalar matrix in an integral (resp. rational) matrix semigroup is undecidable where  $k \in \mathbb{Z} \setminus \{0, \pm 1\}$  (resp.  $k \in \mathbb{Q} \setminus \{0, \pm 1\}$ ), (see [4]).

We shall now show that the membership problem in  $2 \times 2$  unitary quaternion matrix semigroups is undecidable. The proof uses a new approach of encoding PCP proposed in [4]. The main idea is to store all words of the PCP separately and use an index coding to ensure they are multiplied in the correct way.

**Theorem 5.** Given a unitary quaternion matrix semigroup  $S$  which is generated by  $X = \{X_1, X_2, \dots, X_n\} \subseteq \mathbb{H}(\mathbb{Q})^{2 \times 2}$ , it is undecidable for a matrix  $Y$  whether  $Y \in S$ .

**Proof.** Given an instance of the PCP  $(h, g)$  where  $h, g : \Gamma^* \mapsto \Sigma^*$ . Then  $w \in \Gamma^+$  is a solution to the PCP iff  $h(w) = g(w)$ . Assume now that  $\forall x \in \Gamma^*$ ,  $g(x)$  has an inverse,  $g(x)^{-1}$ . In terms of words over  $\Sigma$ , this means that if  $g(x) = y$  for some  $y \in \Sigma^*$  then  $g(x)^{-1} = y^{-1}$  where  $y^{-1} \in \bar{\Sigma}^*$  where  $\bar{\Sigma}$  is a new alphabet containing the inverse of each element of  $\Sigma$ . Formally we say  $a \in \Sigma \Leftrightarrow a^{-1} \in \bar{\Sigma}$ .

For example, if  $g(w) = aabab$  where  $w \in \Gamma^+$  and  $aabab \in \Sigma^*$  then  $g(w)^{-1} = (aabab)^{-1} = b^{-1}a^{-1}b^{-1}a^{-1}a^{-1} \in \bar{\Sigma}^*$ .

If there exists a solution to the PCP,  $w \in \Gamma^+$ , such that  $h(w) = g(w)$  then it can be observed that  $h(w) \cdot g(w)^{-1} = \varepsilon$ . We shall give an example of this simple fact. Let  $w = w_1 w_2 \dots w_k \in \Gamma^+$  be a solution to the PCP. Then  $h(w) = g(w) = u$  for some  $u = u_1 u_2 \dots u_m \in \Sigma^+$ . It is now clear that  $h(w) \dots g^{-1}(w) = (u_1 u_2 \dots u_m) \dots (u_m^{-1} u_{m-1}^{-1} \dots u_1^{-1}) = \varepsilon$ .

This allows us to calculate the solution to the PCP instead as a single word. For each new symbol  $a \in \Gamma$  we wish to add to the existing word  $w \in \Gamma^*$ , we concatenate  $h(a)$  to the left and  $g(a)^{-1}$  to the right of the current word  $v \in \Sigma^*$ , i.e.  $v' = h(a) \cdot v \cdot g(a)^{-1}$ . A solution then exists iff  $v' = \varepsilon$  after a positive number of steps.

Within a semigroup this constraint is difficult to impose; we cannot say “multiply to the left by  $U_i$  and the right by  $V_i$ ”. Such a constraint is possible however by encoding two words simultaneously. In the first word we store the main word corresponding to the PCP itself such as described above. In the second word, we store the index of the word or its inverse.

Given some  $a_i \in \Gamma$ , we define two matrices in the semigroup generator  $Y_{i1}, Y_{i2}$  corresponding to this symbol. In  $Y_{i1}$  we store the two words  $h(a_i)$  and  $\sigma(i)$  where  $\sigma$  is an injective morphism for each  $i \in \mathbb{Z}^+$ ,  $\sigma(i) = a^i b$  where  $a, b \in \Sigma$ . In  $Y_{i2}$ , we store the two words  $g(a_i)^{-1}$  and  $\mu(i)$  where  $\mu(i) = \bar{a}^i \bar{b}$  ( $\bar{a} = a^{-1}$ ,  $\bar{b} = b^{-1}$ ).

We need to store two words separately in one matrix. Let  $\Gamma = \{a_1, a_2, \dots, a_m\}$  and  $(h, g)$  be an instance of the PCP. Then for each  $1 \leq i \leq m$ , define

$$Y_{i1} = \begin{pmatrix} \gamma(h(a_i)) & 0 \\ 0 & \gamma(\sigma(i)) \end{pmatrix}, \quad Y_{i2} = \begin{pmatrix} \gamma(g(a_i))^{-1} & 0 \\ 0 & \gamma(\mu(i)) \end{pmatrix}.$$

Note that all quaternions used are unit. Now define two special matrices:

$$M = \begin{pmatrix} \gamma(h(a_1)) & 0 \\ 0 & \gamma(b) \end{pmatrix}, \quad N = \begin{pmatrix} \gamma(g(a_1))^{-1} & 0 \\ 0 & \gamma(b)^{-1} \end{pmatrix}.$$

We store the mapping of symbol  $a_1$  in  $M, N$ , using the modified PCP to ensure that if there is a solution then there exists a solution using this symbol first. This avoids the pathological case of a product with only  $M$  and  $N$  in it. The matrices  $M, N$  will be used to split the solution into two distinct parts (or a permutation of such a product). One part stores the word connected with morphism  $h$  and the other stores words connected with morphism  $g$ . It's not difficult to see that for any  $i, j \in \mathbb{N}$  then  $|\sigma(i)\mu(j)| = |\sigma(i)| + |\mu(j)|$  and thus if we have  $\varepsilon$  in the lower right of a matrix, we must have used  $M$  or  $N$  at least once. See [4] for fuller details of the construction.

Note that if matrix  $N$  appears once in a product equal to  $I_2$  then matrix  $M$  appears once also due to the above construction. (For the bottom right element to equal 1,  $\gamma(b)$  must multiply with  $\gamma(b)^{-1}$  at some point, see also [12].) Thus if we consider a semigroup,  $S$ , generated by  $\{Y_{i1}, Y_{i2}, M\}$  where  $1 \leq i \leq m$ , then  $N^{-1} \in S$  iff the instance of PCP has a solution, thus membership is undecidable. All matrices are diagonal and unitary quaternion matrices which are equivalent to *double quaternions*. Thus the membership for a semigroup of double quaternions is undecidable.  $\square$

**Corollary 6.** *The vector reachability problem for a semigroup of  $2 \times 2$  quaternion matrices is undecidable.*

**Proof.** The vector reachability question for quaternion matrices is defined as: “Given two vectors  $a, b \in \mathbb{H}(\mathbb{Q})^n$  and a finitely generated semigroup of matrices  $S \subset \mathbb{H}(\mathbb{Q})^{n \times n}$ , does there exist some  $M \in S$  such that  $Ma = b$ ?”. The undecidability is straightforward from the Theorem 5. Let  $x, y \in \mathbb{H}(\mathbb{Q})^2$  and  $x = (1, 1)^T, y = N^{-1}(1, 1)^T$ . Then, for some  $R \in S$ , it is clear that  $Rx = y$  iff  $R = N^{-1} = Y$  since we use only diagonal matrices. Since determining if  $Y \in S$  is undecidable, the vector reachability problem is undecidable.  $\square$

The next problem was given as an open problem over matrices of natural numbers  $\mathbb{N}$  in any dimension [7]. We show it is undecidable over  $\mathbb{H}(\mathbb{Q})^{2 \times 2}$ .

**Theorem 7.** *It is undecidable for a finitely generated semigroup  $S \subseteq \mathbb{H}(\mathbb{Q})^{2 \times 2}$  whether there exists any diagonal matrix  $D \in S$ .*

**Proof.** As before, let  $h, g : \Gamma^* \mapsto \Sigma^*$  be an instance of the PCP where  $|\Sigma| = 2$ . We use the morphisms  $\rho, \tau : \Gamma^* \mapsto \mathbb{H}(\mathbb{Q})$  defined for any  $w \in \Gamma^*$  as  $\rho(w) = \gamma(h(w))$  and  $\tau(w) = \gamma(g(w))$ . Thus  $u, v \in \Gamma^*$ ,  $\rho(u) = \tau(v)$  iff  $u = v$ . For any two quaternions  $q, r \in \mathbb{H}(\mathbb{Q})$  we define

$$\Psi(q, r) = \frac{1}{2} \begin{pmatrix} q + r & q - r \\ q - r & q + r \end{pmatrix}.$$

It is clear that this is still homomorphic [8], since  $\Psi(q_1, r_1) \cdot \Psi(q_2, r_2) = \Psi(q_1 q_2, r_1 r_2)$  which is verified easily via:

$$\frac{1}{2} \begin{pmatrix} q_1 + r_1 & q_1 - r_1 \\ q_1 - r_1 & q_1 + r_1 \end{pmatrix} \cdot \frac{1}{2} \begin{pmatrix} q_2 + r_2 & q_2 - r_2 \\ q_2 - r_2 & q_2 + r_2 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} q_1 q_2 + r_1 r_2 & q_1 q_2 - r_1 r_2 \\ q_1 q_2 - r_1 r_2 & q_1 q_2 + r_1 r_2 \end{pmatrix}.$$

It is now obvious that  $\Psi(u, v)$  is diagonal iff  $u = v$  since the top right and bottom left elements of the matrix equal 0 only if the two quaternions are equal.

Thus we can create one such matrix for each pair of images of letters from  $\Gamma$  using  $\tau$  and  $\rho$ .  $S$  contains a diagonal matrix iff a PCP solution exists.

Unfortunately this does not hold when we convert the matrices to four-dimensional rational matrices since we only get a *block diagonal* matrix. Thus the decidability for whether any matrix in a semigroup is diagonal remains open for integers, rationals and complex rational numbers.  $\square$

Another problem which can be stated is that of *freeness* of quaternion matrix semigroups. We use an almost identical proof to that in [9] to show undecidability, but we obtain the result for matrices over  $\mathbb{H}(\mathbb{Q})^{2 \times 2}$  rather than  $(\mathbb{Z}^+)^{3 \times 3}$ .

**Theorem 8.** *Given a quaternion matrix semigroup  $S$ , which is finitely generated by  $M = \{M_1, \dots, M_n\} \subset \mathbb{H}(\mathbb{Q})^{2 \times 2}$ , deciding whether  $S$  is free is algorithmically undecidable.*

**Proof.** Since we can store two words within a matrix  $M_i \in \mathbb{H}(\mathbb{Q})^{2 \times 2}$  we can use an almost identical proof that was used in [9]. We will give very brief sketch of the proof and refer to [9] for details.

The mixed modification PCP (or MMPCP) is a variant of the standard Post correspondence problem. As in the original PCP, we are given two (finite) alphabets  $\Sigma, \Delta$  and two morphisms  $h, g : \Sigma^+ \rightarrow \Delta^+$ . The MMPCP asks whether there exists a word  $w = w_1 w_2 \dots w_m \in \Sigma^+$  such that:

$$h_1(w_1)h_2(w_2) \dots h_m(w_m) = g_1(w_1)g_2(w_2) \dots g_m(w_m)$$

where each  $h_i, g_i \in \{h, g\}$  and  $h_j \neq g_j$  for some  $1 \leq j \leq m$ . Now, define the set of  $2 \times 2$  quaternion matrices:

$$M = \left\{ \begin{pmatrix} \gamma(a) & 0 \\ 0 & \gamma(h(a)) \end{pmatrix}, \begin{pmatrix} \gamma(a) & 0 \\ 0 & \gamma(g(a)) \end{pmatrix}; a \in \Sigma \right\}$$

and it can be seen that if  $S$  is not free then there is a word  $w = w_1 w_2 \dots w_n \in \Sigma^+$  such that  $h_1(w_1)h_2(w_2) \dots h_m(w_m) = g_1(w_1)g_2(w_2) \dots g_m(w_m)$  since any equal matrix product in  $S$  must have the same word  $w$  in the top left element and the same element in the bottom right which was generated by *different* matrices. Thus the problem of freeness for  $2 \times 2$  rational quaternion matrix semigroups is undecidable. See [9] for fuller details of the proof method.

Note that an alphabet size of  $|\Sigma| = 7$  was required for the undecidability of MMPCP (see [12]), thus the problem is undecidable for 7 matrices.  $\square$

We now consider a problem which is *decidable* over complex numbers, but *undecidable* over rational quaternions. This gives a bound between the computational power of complex numbers and quaternions. We first state the following important theorem.

**Theorem 9.** [2] *Let  $A_1, A_2, \dots, A_k, B_1, B_2, \dots, B_m \in \mathbb{F}^{n \times n}$  be commuting square matrices over an algebraic number field  $F$  and  $A, B \in \mathbb{F}^{n \times l}$ . Determining whether there exists  $i_1, \dots, i_k, j_1, \dots, j_m \geq 0$  such that:*

$$\left( A_1^{i_1} A_2^{i_2} \dots A_k^{i_k} \right) A = \left( B_1^{j_1} B_2^{j_2} \dots B_m^{j_m} \right) B,$$

can be (constructively) solved in polynomial time for fixed  $m$  and  $k$ .

**Corollary 10.** *The problems for diagonal matrices stated in Theorems 3, 4 and 5 are decidable when taken instead over any field up to the complex numbers.*

**Proof.** In Theorem 3, assume no elements are zero (this case is trivial), then for each  $1 \leq i \leq n$  let us define  $c_i = a_i b_i^{-1}$ . Now the problem becomes: does there exist  $r_1, r_2, \dots, r_n \geq 0$  such that  $c_1^{r_1} c_2^{r_2} \dots c_n^{r_n} = 1$  since complex numbers commute. This is decidable by Theorem 9 (setting  $A_i = c_i, B_1 = A = B = 1$  and  $m = 1$ ).

For Theorem 4, we see that complex diagonal matrices commute, therefore we may again use Theorem 9 (using  $A_1, \dots, A_n$  and  $B_1, B_2$  as input and  $A = B = I$  where  $I$  is the identity matrix). The decidability for Theorem 5 over complex algebraic matrices can be proved similarly by inputting  $A_i = X_i, 1 \leq i \leq n, B_1 = I, A = I, B = Y, k = n$  and  $m = 1$ .  $\square$

### 3.1. Computational problems in Lipschitz integers

We also consider decision problems on the *Lipschitz integers* denoted by  $\mathbb{H}(\mathbb{Z})$  which are quaternions with integral parts.

**Corollary 11.** *The problems stated in Theorems 3 and 4 are undecidable when taken instead over the Lipschitz integers  $\mathbb{H}(\mathbb{Z})$ .*

**Proof.** Note that in Lemma 1 we showed  $\gamma$  is injective and in Section 2.2 we showed an isomorphism between quaternions and a subgroup of the two-dimensional complex matrices,  $\mathbb{H}(\mathbb{Q}) \cong \mathbb{C}^{2 \times 2}$ . If we examine the definition of  $\zeta$  in Section 2.2 we see that all elements have 5 as their denominator thus we can multiply  $\zeta(a), \zeta(b)$  by the scalar matrix with element 5 thus giving two-dimensional matrices over the Gaussian integers. This will still be free and is equivalent to the (non-unit) quaternions  $q_1 = 5(\frac{3}{5}, \frac{4}{5}, 0, 0) \cdot \mu = (3, 4, 0, 0) \cdot \mu$  and  $q_2 = 5(\frac{3}{5}, 0, \frac{4}{5}, 0) \cdot \mu = (3, 0, 4, 0) \cdot \mu$  which will now form a free semigroup. We therefore define  $\lambda : \Sigma^* \mapsto \mathbb{H}(\mathbb{Z})$  by

$$\lambda(x) = \begin{cases} 5 \cdot \gamma(x) & \text{if } x \neq \varepsilon \\ \gamma(x) & \text{if } x = \varepsilon \end{cases}$$

Thus in Theorems 3 and 4 we can replace the definitions of  $\rho, \tau$  to use  $\lambda$  and this will give a free morphism over the Lipschitz integers  $\mathbb{H}(\mathbb{Z})$ . This cannot be extended to Theorem 5 since the inverse of a non-identity Lipschitz integer is not itself a Lipschitz integer (obviously it must have rational coefficients).  $\square$

**Theorem 12.** *Given a set of Lipschitz integers  $S \in \mathbb{H}(\mathbb{Z})$  forming a semigroup  $\langle S, \cdot \rangle$ , the problem of deciding for an arbitrary  $L \in \mathbb{H}(\mathbb{Z})$  if  $L \in \langle S, \cdot \rangle$  is decidable.*

**Proof.** Note that all non-zero quaternions have modulus  $d \in \mathbb{R}^+$ . Furthermore, it is obvious that for any non-zero Lipschitz integer  $L \in \mathbb{H}(\mathbb{Z})$ , that  $d \geq 1$ , with equality iff  $L \in \Phi = \{(\pm 1, 0, 0, 0) \cdot \mu, (0, \pm 1, 0, 0) \cdot \mu, (0, 0, \pm 1, 0) \cdot \mu, (0, 0, 0, \pm 1) \cdot \mu\}$ . We have named this set for ease of explanation.

For all  $q \in \Phi$ ,  $q$  is of unit length i.e.  $\|q\| = q\bar{q} = \sqrt{a^2 + b^2 + c^2 + d^2} = 1$ . It can be also noted that their fourth powers are all equal to the identity element:  $\forall q \in \Phi, q^4 = \vartheta_1 = (1, 0, 0, 0) \cdot \mu$  which is easily checked.

For a given  $L$  whose membership in  $S$  we wish to check, it will have a magnitude  $\|L\| = m \in \mathbb{R}$ . If  $m < 1$  then  $L$  cannot be a product a Lipschitz integers since the modulus must be at least 1 by definition of the quaternion modulus. If  $m = 1$  then  $L$  can only be a product of elements from  $\Phi$  and membership is trivial. Otherwise,  $m > 1$ . Let  $S' = S \setminus \Phi$  (i.e. the generator set  $S$  minus any elements of  $\Phi$ ). We can see that there exists only a finite number of products to check since  $m > 1$  and for all  $x \in [S']$  we have that  $\|x\| > 1$ .

Thus, excluding  $\Phi$  we have a finite set of products of finite length to check. However if a (non-identity) element of  $\Phi$  is in the generator, we must include these in the products. For each product  $P = p_1 p_2 \cdots p_n \in S'$  whose magnitude equals  $m$ , i.e.  $\|P\| = m$ , we define the set of products:

$$\left\{ P = \left( \prod_{t=1}^n r_t p_t \right) r_{n+1} \mid r_t, p_t \in \mathbb{H}(\mathbb{Z}) \right\},$$

where each  $r_t$  varies over all elements of  $[(\Phi \cap S) \cup \vartheta_1]$  for  $1 \leq t \leq n + 1$ . We must simply prove that  $[\Phi]$  (the semigroup over elements of  $\Phi$ ) is finite. This is true since the only Lipschitz integers with moduli 1 are in  $\Phi$ , the quaternion moduli is multiplicative and the product of two Lipschitz integers is a Lipschitz integer, all of which are very easy to prove. Thus  $[\Phi]$  is a finite semigroup and there exists a finite set of products to check for equality to  $L \in \mathbb{H}(\mathbb{Q})$  and thus this is a decidable problem.  $\square$

#### 4. Geometric interpretations

In this section, we will move from algebraic point of view to geometric interpretations of quaternion matrix semigroup problems. This leads to an interesting set of problems which we shall now outline.

**Problem 13. Point Rotation Problem (PRP( $n$ ))**—Given points  $x, y \in \mathbb{Q}^n$  on the unit length  $(n - 1)$ -sphere and a semigroup  $S$  of  $n$ -dimensional rotations. Does there exist  $M \in S$  such that  $M$  rotates  $x$  to  $y$ ?

In general, we can consider PRP( $n$ ) with a semigroup of  $n$ -dimensional rotation matrices (i.e. orthogonal matrices with determinant 1). In three-dimensions, we may take  $S$  to be a semigroup of quaternions and define the rotation problem to be  $qx'q^{-1} = y'$  where  $q \in S$  and  $x', y' \in \mathbb{H}(\mathbb{Q})_0$  are pure quaternions with imaginary components corresponding to the vectors  $x, y$ .

We shall show that this problem is *decidable* for two-dimensions. Further, it is *undecidable* in four-dimensions, and its decidability status is open in three-dimensions.

**Theorem 14.** *The Point Rotation Problem PRP(2) is decidable.*

**Proof.** Since the rotation of two-dimensional points is commutative, we can represent the problem as a vector reachability problem with a semigroup  $S \subset \mathbb{Q}^{2 \times 2}$ . Since  $S$  is commutative, we may use the result of Theorem 9 with  $A_i$  being the rotation matrices of the generator of  $S$ ,  $B_1 = I$ ,  $A = x, B = y$ , and  $m = 1$ .  $\square$

**Problem 15. Quaternion Scalar Reachability Problem (QSRP( $n$ ))**—Given vectors  $u, v \in \mathbb{H}(\mathbb{Q})^n$  a scalar  $r \in \mathbb{H}(\mathbb{Q})$  and a semigroup of matrices  $S' \subset \mathbb{H}(\mathbb{Q})^{n \times n}$ . Does there exist  $M \in S'$  such that  $u^T M v = r$ ?

**Theorem 16.** *The Point Rotation Problem PRP(3) is reducible to the Quaternion Scalar Reachability Problem QSRP(2).*

**Proof.** Since we are using three-dimensional rotations, we can convert all elements of the PRP(3) instance to quaternions. We define  $x', y' \in \mathbb{H}(\mathbb{Q})_0$  to be pure quaternions with imaginary parts corresponding to  $x, y$  vectors, respectively. We convert each 3D rotation,  $R$  in  $S$  to an equivalent unit quaternion  $q$  i.e. such that the imaginary vector in  $qx'q^{-1}$  is equivalent to  $Rx$  for example.

Each quaternion  $q$  in the PRP is unit length it is invertible, thus if  $qxq^{-1} = y$  we may write  $qx = yq$ . Let  $G = \{q_0, q_1, \dots, q_m\} = S' \setminus S^2$  be the generator of  $S'$ . Define  $\alpha = (y, 1)$  and  $\beta = (-1, x)^T$  and let  $G' = \{M_0, M_1, \dots, M_m\}$  where  $M_i = \begin{pmatrix} q_i & 0 \\ 0 & q_i \end{pmatrix}$  and let  $T = \langle G', \cdot \rangle$  be a new semigroup. Then there exists  $M \in T$  such that  $\alpha M \beta = 0$  iff  $\exists q \in S$  such that  $qxq^{-1} = y$ . To see this, note that  $\alpha M \beta = qx - yq$  where  $M = \begin{pmatrix} q & 0 \\ 0 & q \end{pmatrix}$  and  $qx - yq = 0 \Rightarrow qx = yq \Rightarrow qxq^{-1} = y$  as required.  $\square$

In fact we know that QSRP(2) is undecidable in general:

**Theorem 17.** Quaternion Scalar Reachability Problem is undecidable for a semigroup  $S$  generated by 5 two-dimensional diagonal quaternion matrices.

**Proof.** Let  $\gamma : \Sigma^* \mapsto \mathbb{H}(\mathbb{Q})$  be defined as previously. Given a Claus instance of PCP,  $\{(u_1, v_1), (u_2, v_2), \dots, (u_n, v_n)\} \subseteq \Sigma \times \Sigma$ , then we see that if

$$M_i = \begin{pmatrix} \gamma(u_i) & 0 \\ 0 & \gamma(v_i) \end{pmatrix}$$

for each  $2 \leq i \leq n - 1$  and  $\alpha = (\gamma(u_1), \gamma(v_1))$ ,  $\beta = (\gamma(u_n), -\gamma(v_n))^T$  then:

$$\alpha M_w \beta = \gamma(u_1 u_w u_n) - \gamma(v_1 v_w v_n) = 0 \Leftrightarrow u_1 u_w u_n = v_1 v_w v_n$$

where  $M_w = M_{w_1} M_{w_2} \dots M_{w_k}$  and  $1 \leq w_i \leq n - 1$  for each  $1 \leq i \leq k$ . Since there exists a Claus instance of PCP which is undecidable for  $n = 7$  [12], the problem is undecidable for 5 matrices (putting the first and last elements inside  $\alpha, \beta$ ).  $\square$

But the decidability status of PRP(3) remains open (since the reduction is one way). We next show that PRP(4) is undecidable.

**Theorem 18.** The Point Rotation Problem PRP(4) is undecidable.

**Proof.** The set of all unit quaternions forms a three-dimensional sphere (3-sphere) and any pair of unit quaternions  $a$  and  $b$  can represent a rotation in 4D space. We can rotate a point  $x = (x_1, x_2, x_3, x_4)$  on the 3-sphere, represented by a quaternion  $q_x = (x_1, x_2, x_3, x_4)$ , in the following way:  $aq_x b^{-1}$ .

Given a finite set of rotations,  $\{(a_1, b_1), \dots, (a_n, b_n)\}$ , represented by pairs of quaternions. The question of whether a point  $x$  on the 3-sphere can be mapped to itself by the above set of rotations is equivalent to the problem whether there exists a non-empty sequence of indices  $(r_1, \dots, r_m)$  such that  $a_{r_1} \dots a_{r_m} q_x b_{r_m}^{-1} \dots b_{r_1}^{-1} = q_x$ .

If  $x$  is a point represented by quaternion  $(1, 0, 0, 0) \cdot \mu$ , then the above equation only holds when  $a_{r_1} a_{r_2} \dots a_{r_m} = b_{r_1} b_{r_2} \dots b_{r_m}$ . According to Theorem 3 we have that the four-dimensional Point Rotation Problem is undecidable for 7 rotations. Moreover it is easy to see that PRP(4) is undecidable even for 5 rotations using the idea of Claus instances of PCP [12] where two of the rotations (the first and the last one) can be fixed and used only once.  $\square$

**Corollary 19.** The vector reachability problem for  $n \times n$  rational orthogonal matrix semigroups is decidable when  $n \leq 2$  and undecidable for  $n \geq 4$  with at least 5 matrices in the semigroup generator.

**Open problem 1.** Given a semigroup of rational quaternions,  $S$ , generated by a finite set  $Q \subset \mathbb{H}(\mathbb{Q})$ , is membership decidable for  $S$ ? That is, can we decide if  $x \in S$  for any  $x \in \mathbb{H}(\mathbb{Q})$ ? Also, is the freeness of semigroup  $S$  decidable?

A related open problem mentioned above can also be stated:

**Open problem 2.** Given two points on the 2-sphere,  $x, y \in \mathbb{Q}^3$ , and a semigroup of rotations  $S$  generated by a finite set  $G$ . Does there exist an algorithm to determine whether there exists a rotation  $R \in S$  such that  $R$  rotates  $x$  to  $y$ ?

The rotation problem PRP(3) is not only related to problems on quaternions but can also be reformulated as a one-dimensional vector reachability problem for a semigroup or a group of rational linear functions over the complex field also known as Möbius transformations. In geometry, a Möbius transformation is a function,  $f : \mathbb{C} \mapsto \mathbb{C}$  defined by:

$$f(z) = \frac{az + b}{cz + d},$$



where  $z, a, b, c, d \in \mathbb{C}$  are complex numbers satisfying  $ad - bc \neq 0$ . Möbius transformations may be performed by taking a stereographic projection from a plane to a sphere, rotating and moving the sphere to a new arbitrary location and orientation, and making a stereographic projection back to the plane. Since there is a unique mapping between rotations of the 2-sphere and Möbius transformations, problem *PRP(3)* is equivalent to the reachability problem of non-deterministic iterative maps: “Given a finite set  $M$  of one-dimensional linear rational functions over the complex field and two points  $x$  and  $y$  on the complex plane. Does there exist an algorithm to determine whether it is possible to map  $x$  to  $y$  by a finite sequence of linear rational functions from the set  $M$ ?”.

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