Forming groups with 4 × 4 matrices

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The three Pauli matrices are normally given [1] as the 2 × 2 matrices:

$$a = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad b = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad c = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where 'i' is the usual complex number imaginary unit.

These matrices obey the relations $a^2 = I = b^2 = c^2$ (where I is the 2 × 2 identity matrix), as well as the anticommutation relations:

$$bc = -cb = ia,$$

$$ca = -ac = ib,$$

$$ab = -ba = ic.$$

Within the quantities ia, ib and ic, i is a scalar multiplier of the 2 × 2 Pauli matrices and, of course, commutes with each of a, b, c.

It is noted that in complex number theory [2] the general complex number $a + ib$ $(a, b \in \mathbb{R})$ can be given as $\begin{pmatrix} a & -b \\ b & a \end{pmatrix}$.

In this format, 2 × 2 matrices form a field that is isomorphic to the set of complex numbers. The element i is represented as $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$ and i^2 is $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$, the negative unit matrix. This is all well known so far!

The Pauli matrices can be readily expanded to become a set of three 4 × 4 matrices containing only *real* entries from the set $\{-1, 0, 1\}$. The i within the Pauli b matrix is replaced by $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$.

Rewriting a, b and c as 2 × 2 partitioned matrices:

$$a = \left(\begin{array}{c|c} 0 & 1 \\ \hline 1 & 0 \end{array}\right); \quad b = \left(\begin{array}{c|c} 0 & -i \\ \hline i & 0 \end{array}\right); \quad c = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -1 \end{array}\right).$$

We can replace the entries 0; 1; −1; i by the respective 2 × 2 matrices $\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$; $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$; $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$; $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, giving 4 × 4 representations:

$$a = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}; \quad b = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}; \quad c = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

If i is now represented by $\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$ it is found that i^2 gives the negative 4×4 unit matrix and *all the relations* for the Pauli matrices *still hold*. So that

$$\begin{cases} a^2 = I = b^2 = c^2 \\ bc = -cb = ia \\ ca = -ac = ib \\ ab = -ba = ic \end{cases} \qquad \text{[all symbols used are } 4 \times 4 \text{ matrices].}$$

We would like to make the point that there are possibly several representations for i (as a 4×4 matrix). The one chosen above is a 'natural' one as it is derived from the general quaternion matrix (discussed later). The i matrix chosen *commutes* with each of a, b and c (as 4×4 matrices). This would be a basic requirement in quantum physics where i is used as a field element and commutes with all quantities. This commuting property does not necessarily hold for other possible representations for i.

The elements

$$\{I, -I, i, -i, a, b, c, -a, -b, -c, ab, -ab, ca, -ca, bc, -cb\}$$

(where $-ab = ba$, $-ca = ac$, $-bc = cb$), form a *group* of order 16. Each element is a 4×4 matrix. The matrices are each orthogonal. Elements are either self-inverse, e.g. a, b, c, or have their negative as their inverse, e.g. i, ab.

The subgroup consisting of $\{I, -I, i, -i\}$ is *normal* of order 4.

We now examine the representation of quaternions as 4×4 matrices and see how these can be combined with the three Pauli matrices a; b; c.

The general quaternion is represented as a 4×4 matrix [3]

$$\begin{pmatrix} p & -q & -r & -s \\ q & p & -s & r \\ r & s & p & -q \\ s & -r & q & p \end{pmatrix} \text{ where } p, q, r, s \in \mathbb{R}.$$

Normally Hamilton's quaternions are written as $p + qi + rj + sk$ where i, j, k are imaginary units and p, q, r, s are real.

The real part of the quaternion, p, appears on the principal diagonal of the matrix (as does the real part of the familiar complex number $a + ib$ in the 2×2 matrix representation). The quaternions form a division ring—as, it will be seen, do the 4×4 matrix representations.

By setting $p = 0$; $q = 1$; $r = 0$; $s = 0$, we obtain a representation for i. By setting $p = 0$; $q = 0$; $r = 1$; $s = 0$, we obtain j and by setting $p = 0$; $q = 0$; $r = 0$; $s = 1$, we obtain k.

We have now

$$i = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}^{*} \quad j = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \quad k = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$

It can be verified that all the Hamilton relations among i, j, k hold with these matrices:

$$\begin{array}{lll} i^2 = -I \; ; & ij = k \; ; & ij = -ji \; ; \\ j^2 = -I \; ; & jk = i \; ; & jk = -kj \; ; \\ k^2 = -I \; ; & ki = j \; ; & ki = -ik \; . \end{array}$$

i, j, k anticommute in pairs in similar fashion to the three Pauli matrices a, b, c.

We note that i, j, k can be combined with (multiplied with) a, b, c. It has already been mentioned that i commutes with each a, b, c but, remarkably, the j matrix and the k matrix *anticommute* with each of a, b, c. We now have the relations:

$$\begin{array}{lll} ia = ai \; ; & ja = -aj \; ; & ka = -ak \; ; \\ ib = bi \; ; & jb = -bj \; ; & kb = -bk \; ; \\ ic = ci \; ; & jc = -cj \; ; & kc = -ck \; . \end{array}$$

[From above, we already have $ia = bc$; $ib = ca$; $ic = ab$.]

By grafting the six matrices: ja, jb, jc, ka, kb, kc and their negatives $-ja$, $-jb$, $-jc$, $-ka$, $-kb$, $-kc$ onto the 16 elements (as discussed above), we obtain 28 elements. By, including j and k themselves, with their negatives $-j$ and $-k$, we obtain exactly 32 elements (exactly *double* the order of the group discussed previously) which will form a group of order 32.

The set of elements is:

$$\begin{array}{llllllllllllll} \{ \; I, & -I, & i, & -i, & j, & -j, & k, & -k, & a, & b, & c, & -a, & -b, & -c, \\ ab, & ba, & ca, & ac, & bc, & cb, & ja, & -ja, & jb, & -jb & jc, & -jc & & \\ & & & & & & ka, & -ka, & kb, & -kb, & kc, & -kc & \} & \end{array}$$

Associativity of elements holds because all matrices obey this property. All elements are self-inverse *or* have their negative as inverse—the same as for the 16 element group above. In fact, the 32 element group has the 16 element group as a normal subgroup within it. As well as this, the 8 elements $\{I, -I, i, -i, j, -j, k, -k\}$ form another normal subgroup of the 32 element one (though it is *not* a subgroup of the 16 element group).

The 8 element subgroup is the familiar 'quaternion group'. It should be mentioned here that some textbooks, notably [4], present this group in a rather indirect way.

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* as cited above.

On the closure property of the 32 element group, we feel this is an excellent exercise, checking that pairs multiplied together give another in the set. For example:

(1) $$(a) \times (ja) = (aj) \times (a) = (-ja) \times (a) = -j(a \times a) = -jI = -j$$

(2) $$(ab) \times (jc) = (ic) \times (jc) = i \times (cj) \times c = i \times (-jc) \times c = -ij \times c^2 = -k \times I = -k.$$

Some striking results have arisen by combining the 4 × 4 Pauli matrices with the 4 × 4 quaternion units:

1) All groups formed have order 2^N for $N = 2, 3, 4, 5$. Further to this, if N is an *odd* power, $(2^3, 2^5)$, the group contains all of i, j, k. Whereas if N is an *even* power, $(2^2, 2^4)$, the group contains only the i element with a, b, c. This shows that the 2^5 (or 32) element group is an extension of the 2^3 (or 8) element quaternion group.
2) All the 4 × 4 matrix elements are *orthogonal matrices*. (The transpose of each matrix gives its inverse.)
3) Any subgroups of a given group are *normal* (*invariant* in some textbooks) and thereby further groups, such as *quotient groups*, could be created.
4) The fact that the *five* quantities $\{a, b, c, j, k\}$ *anticommute*, for any pair selected, is significant as this value five occurs with the 5 Dirac matrices in quantum physics. Any pair from the 5 Dirac matrices anticommute [1].
5) The fact that j and k each anticommute with a, b, c (and *not* i) suggests a *symmetry breaking* of the units i, j, k. This is perhaps a surprising result as Hamilton's relations between i, j, k are cyclically symmetric.

References

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