Quaternions and the Heuristic Role of Mathematical Structures in Physics

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Abstract

One of the important ways development takes place in mathematics is via a process of generalization. On the basis of a recent characterization of this process we propose a principle that generalizations of mathematical structures that are already part of successful physical theories serve as good guides for the development of new physical theories. The principle is a more formal presentation and extension of a position stated earlier this century by Dirac. Quaternions form an excellent example of such a generalization, and we consider a number of the ways in which their use in physical theories illustrates this principle.

Key words: Quaternions, heuristics, mathematics and physics, quaternionic quantum theory.
1 Introduction

In recent decades the necessary role mathematical structures play in the formulation of physical theories has been the subject of ongoing interest. Wigner’s reference in a well known essay of 1960 to the “unreasonable effectiveness” of mathematics in this role has captured what is undoubtedly a widespread feeling that this success is remarkable, and moreover, in need of further explanation. Wigner himself noted that this role of mathematics is a “wonderful gift we neither understand nor deserve.” The topic has been of interest not only to physicists and mathematicians, but also to those working on the philosophical implications and foundations of both subjects.\footnote{The recent collection of essays in Ref. \cite{2} provides a guide to the literature as well as an introduction to the variety of ways in which this topic may be approached. Other recent discussions may be found in Refs. \cite{3, 4, 5, 6}.}

Much of the discussion on this topic has focused on particular physical theories and sought to explore what one may infer about the nature of either mathematical or physical knowledge or the entities of concern to both disciplines from the role of mathematics in these theories. Mathematics, however, also plays an important role in the development of new physical theories, and while less attention has been paid to this heuristic role of mathematics, its importance has been well recognized. In a series of essays Bochner, for example, has traced significant episodes in the development of physics where mathematics has played a crucial role, and in recent studies Redhead and Zahar have identified in a formal manner a number of ways in which this may take place. In this essay we wish to propose a way in which mathematics may play such a heuristic role in physics which is not explicitly mentioned in these works, although an implicit recognition of it may be found in the work of Bochner. In particular we wish to draw attention to the importance of certain developments within mathematics itself for the development of new physical theories.\footnote{\cite{7, 8, 9, 10}}
of physics.

Unlike the situation in the natural sciences, a concern with the particular manner in which mathematics evolves has been of relatively recent origin. The works of Crowe [1], Koppelman [12] and Wilder [13, 14], for example, which aim at characterizing the nature of mathematical evolution, only stem from the late sixties. Of even more recent origin are the works on this topic by Hallet [15], Kitcher [16], and others [17, 18] within the philosophy of mathematics. In these works the ideas of philosophers such as Kuhn and Lakatos have been used to explore both the question of progress and the “logic of discovery” in mathematics as well as the parallels between the development of mathematics and science.

In this essay we wish to exploit a characterization given by Kitcher [16] of one of the important ways mathematics progresses, which he identifies as one of “generalization.” This refines an idea stated by Dirac in 1931 on the manner in which certain developments in mathematics can play an important heuristic role in physics. In particular, we wish to propose that generalizations of those mathematical structures of physical theories which at any stage enjoy a measure of success in describing nature supply new mathematical structures that can serve vital roles in the development of new physical theories. In addition, we propose that through their use in this manner better understanding of present theories is obtained which in turn can give a good base for the development of new theories. In Section 2 we will provide a characterization of generalization which will flesh out this position, and we will provide some examples of where it has occurred in the development of physics. Dirac’s statement of the idea occurs in his famous essay of 1931 on the quantized singularities in the electromagnetic field.2

2 The idea can also be found in general articles by Dirac in Refs. [11, 20]. In Ref. [19] Dirac notes that a “powerful new method” for the physicist consists of choosing a branch of mathematics and then proceeding “to develop it along suitable lines, at the same time looking for that way in which it appears to lend itself naturally to physical interpretation.” While mention
The most powerful method of advance that can be suggested at present is to employ all the resources of pure mathematics in attempts to perfect and generalize the mathematical formalism that forms the existing basis of theoretical physics, and after each success in this direction, to try to interpret the new mathematical features in terms of physical entities… [21]

Naturally, the task of interpreting the new mathematical structures and forming a physical theory using the structures is an all important and difficult one, however, our focus in this essay is on the importance of exploiting certain types of mathematical developments. In addition, the statement of our position in the next section must of necessity be somewhat informal. Non-trivial generalizations in mathematics require creative insights that by their nature defy prediction, and moreover, there is no guarantee that all possible generalizations of the structures in use at any one time in physics might be of relevance to new physical theories. Our investigation of the natural world is such that we have no well-defined algorithm for generating new scientific theories. Nevertheless, there is good historical evidence that mathematical structures of the sort indicated above are indeed productive in the development of new physical theories.

We should mention that others have expressed ideas similar to the one of Dirac we have mentioned above. Whitehead [22], for example, writing on the role of mathematics in science around the same time as Dirac noted a similar phenomenon in the manner in which the growth of modern physics depended very much on advances towards abstraction in mathematics:

is made in Ref. [20] of the need for a “higher and higher” mathematics no mention is directly made of “generalization” in either article. Instead “mathematical beauty” is mentioned as one of the criteria for deciding on appropriate mathematical developments. Beauty in mathematics, however, is notoriously difficult to define, while the notion of “generalization” is more amenable to specification.
Nothing is more impressive than the fact that as mathematics withdrew increasingly into the upper regions of very greater extremes of abstract thought, it returned back to earth with a corresponding growth of importance for the analysis of concrete fact. . . . The paradox is now fully established that the utmost abstractions are the true weapons with which to control our thought of concrete fact.\footnote{Ref. \cite{22}, p. 47.}

The concept of generalization which we will outline in Section 2 is not unlike the process of abstraction Whitehead is referring to, and moreover, our proposal maintains in a similar manner to Whitehead the idea that mathematical developments of this nature are the ones best able to capture the particularity of our world.

In Sections 3–4 of our essay this position will be explored for the particular “test case” example of quaternions. Quaternions were discovered by Hamilton in 1843. They form an associative division algebra of which the only other members are the real and complex numbers. They provide an excellent example of the type of mathematical generalizations of concern to us, and furthermore, they are generalizations of complex and real numbers, numbers which play central roles in current physical theories. The history of the attempts to use them in physical theories is both interesting and marked with controversy, and as Gürsey \cite{23} has observed, forms an interesting episode in the relationship between mathematics and physics.

We will argue that while quaternions at the moment do not have an assured a place in physical theories as do the other two associative division algebras, there are a number of interesting senses in which they do illustrate our principle. Our treatment of quaternions is not intended to be comprehensive as the history of their use in physics has been well covered in other places \cite{23}; rather, we will focus
directly on aspects related to our argument concerning the role of mathematical structures in physics.

2 Mathematical Generalization and the Development of Physics

2.1 Mathematical Generalization

The patterns evident in mathematical evolution are numerous and complex. Kitcher identifies five types as being of importance for the progress of mathematics one of which is the process of generalization. For Kitcher this process entails several elements: i) it introduces new expressions to the mathematical language; ii) it preserves some features used in the old expressions; iii) in the process certain constraints on prior usage are abandoned; iv) a new theory is obtained with analogues of the old; v) the new structure brings to our attention properties of familiar entities which enables us to see the old theory as a special case. In this way the generalization enables areas already developed to be illuminated in a new way. Kitcher mentions the examples of Hamilton’s creation of quaternions, Lebesgue’s theory of integration, and Cantor’s extension of arithmetic to transfinite numbers as fitting his characterization of generalization.

While Kitcher focuses on characterizing generalizations as evident in the work of given individuals, there is good reason to see many developments in mathematics as fitting this pattern, even though neither at the point of their creation nor in their development by their creator might all of these elements have been evident. For example, it was not until the middle of the nineteenth century, after they had established themselves in algebra and in the theory of complex functions through the geometrical interpretation of Wessel, Argand and Gauss, that complex num-
bers could be seen as generalizations of real numbers in the sense given in i)–v).\[^4\] The development of non-Euclidean geometries can also be seen as a generalization of this sort as well as the developments that arose from the move of “localization” made by Riemann in the study of the geometry of surfaces, and Lie in the study of continuous groups.

With this specification of generalization of a mathematical structure, Dirac’s idea is made more precise. The reasons as to why generalizations of this nature of structures which are currently part of successful physical theories should be of such importance for the development of new physics is an important question, but it is not one we address here. We feel there is sufficient evidence from the actual development of physics to justify such a position, and that a profitable way to go about developing new physical theories will be to proceed in the manner the principle suggests. We choose two particular mathematical structures as illustrations.

### 2.2 Some Illustrations

Our first is pertinent to the theme of the paper and concerns two roles complex numbers have had in the development of physics through their ability to represent phases. Here we view complex numbers as generalizations of real numbers. In a work published in 1831 Fresnel noted that for certain angles of incidence and reflection of polarized light the ratio of the amplitudes is complex but with an absolute value of 1. Fresnel interpreted the ratio to be given by $e^{i\theta}$ with $\theta$ representing the phase shift between the two waves. His result was later experimentally confirmed. Another place where complex numbers play an essential role is in quantum mechanics, and moreover their presence uniquely characterizes im-

\[^4\]Details of this development may be found in Kline’s excellent history of mathematics [24].
portant features of the theory. At the time of the original formulations of both Heisenberg and Schrödinger, their presence posed problems of how to interpret the mathematical formalism of the theory. These were solved by Born’s interpretation of taking $\psi\psi^*$ to represent a probability density. In its most common modern formulation states are represented in a complex vector space, and via their presence as complex phases represent interference phenomena that are unique to quantum states. In addition, as it was recognized very early in the development of quantum theory, electromagnetism could be incorporated into the theory via the complex phases. Thus the feature noted by Argand in 1906 that complex numbers generalize real numbers by adding a concept of rotation has proved to be of extraordinary value in providing an added structure needed for theories such as quantum mechanics.\footnote{For Bochner\footnote{2}, Fresnel’s achievement was the first time physical features were “abstracted” from a purely mathematical structure that had been developed independently of physical considerations. Bochner also clearly notes that complex numbers provide a higher level of abstraction than real numbers. In combination both of these positions can be seen as implying the one we are maintaining here.}

Our second example concerns the important role Lie groups play in physical theories, and we note two places where generalizations within the concept of Lie groups have been important in developing new physical theories. The first was the use of a non-Abelian Lie group by Yang and Mills in 1954 to form a theory built on a generalization of electromagnetic gauge invariance. Thus instead of a single scalar function characterizing the transformation, as in the case of electromagnetism, the functions were members of a non-Abelian group. The work of Yang and Mills has flowered into the current gauge theories of the fundamental interactions. A second place where a generalization has been important has been in the development of supersymmetry theories. These are based on a generalization of the notion of a Lie algebra to a graded Lie algebra\footnote{23}. While there is
no evidence that such a symmetry is realized in nature, supersymmetry theories have many attractive features such as relating spacetime and internal symmetries in a non-trivial manner and providing a Fermi-Bose symmetry.

We are not arguing that these theories proceeded by the deliberate use of mathematics in the sense we are proposing; the complex development evident in all of the above examples reveals a variety of motives and ways of proceeding. It does, however, reveal a pattern in the type of mathematics that can be important in the development of new physical theories. For our principle to have a “force” to it, it is important that all the elements of generalization of Kitcher’s definition be present. For example, some types of mathematical structures generalize others by simply increasing the number of dimensions. Since these need not lead to new expressions that both preserve and relax some of the constraints on the old expression, they need not be a type of generalization that fits Kitcher’s definition, and thus would not be the type of structures with the heuristic role indicated by our position.

3 Quaternions: Nineteenth Century

In this section a number of the significant mathematical developments associated with quaternions during the nineteenth century will first be considered. The degree to which they may be seen to have played any sort of heuristic role in physical developments in that century will then be considered.

3.1 Mathematical developments

Quaternions were discovered by Hamilton in 1843 after more than a decade of attempts to generalize complex numbers to three dimensions. Instead of an entity which he expected to be characterized by three numbers, Hamilton found that
four numbers were required. In modern notation, Hamilton discovered that the form

$$q = q_0 + q_1 e_1 + q_2 e_2 + q_3 e_3$$  \hspace{1cm} (1)$$

with multiplication rules for the “quaternion units” $e_i$ given by,

$$e_i e_j = -\delta_{ij} + \epsilon_{ijk} e_k$$  \hspace{1cm} (2)$$

obeys the same multiplication rules as complex numbers except for commutativity. In equation (2) $\epsilon_{ijk}$ is antisymmetric in the indices with $\epsilon_{123} = \epsilon_{231} = \epsilon_{312} = 1$, and the summation convention is assumed for repeated indices. With these rules the quaternion product has the form

$$p \otimes q = (p_0 q_0 - p_i q_i) + p_0 q_i e_i + p_0 q_i e_i + \epsilon_{ijk} p_i q_j e_k.$$  \hspace{1cm} (3)$$

Hamilton defined a conjugate quaternion by

$$\overline{q} = q_0 - q_1 e_1 - q_2 e_2 - q_3 e_3.$$  \hspace{1cm} (4)$$

With the norm of a quaternion given by

$$N(q) \equiv q \otimes \overline{q} = q_0^2 + q_1^2 + q_2^2 + q_3^2,$$  \hspace{1cm} (5)$$

an important “law of moduli” holds for two quaternions:

$$N(p \otimes q) = N(p) N(q).$$  \hspace{1cm} (6)$$

The law of moduli was of particular importance to Hamilton and it occurs in a notebook entry made on the very day he discovered quaternions. Indeed in a

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\(^6\) Hamilton’s discovery forms one of the well documented discoveries in mathematics. Details may be found in biographies of Hamilton by Hankins \[26\] and O’Donnell \[27\], and in the more specialized studies in Refs. \[28, 29, 30, 31\] \[32, 33, 34\]. For Hamilton’s work see his Lectures on Quaternions \[35\], and the collection of papers pertaining to quaternions in Ref. \[36\].
letter written the day after his discovery he noted that without this property he would have considered the “whole speculation as a failure.” With this property quaternions can be divided and form a division algebra. Scalar and vector parts of a quaternion can be defined as

\[ S_q = \frac{1}{2}(q + \overline{q}), \quad V_q = \frac{1}{2}(q - \overline{q}), \]  

and it may be readily seen that for a product of two “pure quaternions” consisting only of vector parts, the multiplication law in equation (3) contains in one product both the “dot” and “cross” products of the vector analysis that was later to be developed. From the beginning Hamilton was concerned with the geometrical interpretation of quaternions and sought a role for quaternions in describing rotations of pure quaternions. Cayley [37], however, was the first to publish what is now the accepted understanding. If \( R \) is a quaternion of norm 1, then a rotation of \( q \) given by

\[ q' = RqR^{-1}, \]  

leaves \( S_q \) invariant and transforms \( V_q \) according to a rotation about an axis given by the pure vector part of \( R \). In particular if \( R \) is parametrized by

\[ R = \cos \frac{\alpha}{2} + (r_1 e_1 + r_2 e_2 + r_3 e_3) \sin \frac{\alpha}{2} \]  

then the rotation consists of a rotation of \( \alpha \) about an axis determined by the direction of \( (r_1 e_1 + r_2 e_2 + r_3 e_3) \). Cayley noted that the parameterization of the transformation in equation (9) corresponded to that given by Rodrigues in 1840 three years before Hamilton’s discovery of quaternions. Cayley also showed that rotations in a 4-dimensional Euclidean space could be given by quaternions.

\[ \text{As Altmann’s work [28, 29] has clearly revealed, Hamilton mistakenly gave a preference to interpreting quaternions in the form of equation (3) as representing rotations by } \alpha/2 \text{ rather than by } \alpha. \text{ Associated with this interpretation were two further problems of interpretation. First, Hamilton associated the quaternion units, } e, \text{ with } \pi/2 \text{ rotations following the interpretation} \]
In his early writings on quaternions Hamilton also introduced the 3-dimensional "del" operation which he wrote as $\nabla$:

$$\nabla = e_1 \frac{d}{dx} + e_2 \frac{d}{dy} + e_3 \frac{d}{dz},$$

(10)

and noted of its square,

$$-\nabla^2 = \left(\frac{d}{dx}\right)^2 + \left(\frac{d}{dy}\right)^2 + \left(\frac{d}{dz}\right)^2$$

(11)

that "applications to analytical physics must be extensive to a high degree." Until his death in 1865 Hamilton devoted most of his work to developing the mathematical properties of quaternions without, however, considering much in the way of their applications to physics.

Shortly after Hamilton’s discovery of quaternions a generalization to eight units was discovered by Graves and independently by Cayley. These “Octonions” obeyed the “law of moduli” of equation (6) but without the algebraic property of an associative multiplication law. Before the century had closed two important results clarified further the nature of generalizations involved in quaternions and octonions. In 1878 Frobenius [38] proved that the only associative division algebras consist of the real, complex, and quaternion numbers, and in 1898 Hurwitz [39] proved that if associativity is dropped only one further division algebra results, viz., that of the octonions. A further generalization took place when quaternions were shown to be a particular example of order three of Clifford algebras [32]; however, higher orders of Clifford algebras fail to form a division algebra which is the property quaternions share with the real and complex numbers.

8For further details see Ref. [36], p. 263.
In the light of the principle we are proposing here it is interesting to note that for a number of nineteenth century partisans of quaternions that followed Hamilton, such as the Edinburgh physicists Tait and Knott, quaternions were very much seen to be generalizations of previous mathematical structures. Kelland and Tait [40], for example, noted explicitly that quaternions provided “the most beautiful example of extension by the removal of limitations” and noted how room was made for a new understanding of multiplication once the commutativity law was given up by Hamilton. Both of these features correspond to elements of the characterization of generalization given by Kitcher. Furthermore, Kelland and Tait saw these features as reasons to consider the application of quaternions to physics. We note at this point one important aspect of Kitcher’s definition of mathematical generalization that is exemplified by quaternions, namely, since such generalizations both preserve and relax a number of the features of the previous structure they will entail a limited set of new features. It is the limited options available with such particular structures which provides structures of interest for forging new physical theories. We will return to this point later.

3.2 Physical Applications

The main use of quaternions in the nineteenth century consisted in expressing physical theories in the notation of quaternions rather than in Cartesian coordinates. One of the important works where this was done was Maxwell’s *Treatise on Electricity and Magnetism* [41]. As well as presenting equations in Cartesian coordinates in a number of places Maxwell also gave their quaternionic form. Of particular importance was his use of Hamilton’s “del” operator of equation (10). We find no examples where they played a role in the development of new physical theories. While one does find claims, such as those in a textbook by McAulay [12], that new results from existing theories were obtained by the use of quaternions
they were of a relatively minor nature. The importance of the notational role of quaternions, however, should not be underestimated. Again and again those who used quaternions such as Tait and McAulay emphasized that the physical meaning of equations was revealed in a transparent manner when they were expressed in quaternionic form. One finds echoes of this virtue ascribed to quaternions in the nineteenth century also in recent years when mention is made of the value of using coordinate free methods of modern differential geometry in spacetime physics, rather than the older tensor methods.

In addition, the quaternionic formulation, and especially as used by Maxwell in his *Treatise*, did play an important role in the independent development of the vector analysis by Gibbs and Heaviside in the 1880’s. Both Gibbs and Heaviside noted that a formulation of electromagnetism could be given using the separate vector and scalar parts of Hamilton’s quaternions, and moreover, such a formulation proved to be far more accessible for the individual representation of electric and magnetic effects. Heaviside, for one, emphasized what he felt to be the impractical nature of quaternions and when referring to the negative norm for a vector, when taken as part of a quaternion, wrote of the “inscrutable negativity of the square of a vector in quaternions; here, again, is the root of the evil” [45]. The analyses of Stephenson [17], Crowe [30], and Hankins [26] provide details of the important role quaternions played in the later developments of vector analysis. Towards the end of the century the very value of using quaternions at all in physics gave rise to an interesting and rather heated series of exchanges in the journal *Nature* between Tait, McAulay, and Knott on the one side, as supporters of quaternions, and Gibbs and Heaviside on the other. A recent biographer of

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9 For Tait’s comments on this aspect of quaternions see Chapters CXVI and CXVII of his collected works [44] and Ref. [43].
Heaviside [48] has referred to this debate as the “The Great Quaternionic War”. At the end of the century the methods of vector analysis had become standard, and the value of quaternions largely discredited.

Writing in 1943 on the occasion of the centenary of the discovery of quaternions, Whittaker noted that one of the reasons for the demise of the “Hamilton school” consisting of those that sought to make quaternions central in physics, was their failure to continue “that instinct for the generalization of a theory which is characteristic of the mathematician” [33]. Whittaker suggested that people such as Tait and Knott focused more on the “re-writing” of existing theories than on exploiting the significant and unique aspects of quaternions such as their non-commutativity properties. In addition, Whittaker noted, formal mathematical developments related to physical ideas which to some physicists represent “mere mathematical playthings” tend later to come into prominence in physics. One example Whittaker mentioned was the way many of the more mathematical aspects of Hamilton’s work on dynamics have found a place in quantum theory in this century. Whittaker’s comments underline our position in attesting to an aspect of the particular heuristic role we are assigning to mathematics in physics.

4 Quaternions: Twentieth Century

It has only been in this century that unique features of quaternionic structures have been woven closely into the development of new physical theories. Two particular examples which we mention in Section 4.2 are the theories of quaternionic quantum mechanics and supergravity. A number of uses, such as some of the applications to special relativity, do clearly fit the category of “reformulation” of existing theories with claims that the resultant structure possess an elegance and

\footnote{Details of this debate and references to the original literature may be found in Refs. [48, 48].}
aesthetic appeal.

4.1 Mathematical Developments

Three particular mathematical developments associated with quaternions will be mentioned here. All three associate quaternions with other important mathematical structures, and represent a phenomenon in the development of mathematics which the historian of mathematics Wilder [13, 14] has referred to as “consolidation.” When consolidation takes place various structures which were originally separate from each other, and seemingly unrelated, are brought into relationship with each other. The importance for physics resides in presenting various ways in which a generalized mathematical structure may be seen to be related to those within existing theories, and thus may be used in new theories.

The first is the association of quaternions with the Pauli matrices which is mathematically rather insignificant, but of some importance for physics. In the nineteenth century Cayley had given a matrix representation of quaternions, but one important realization of the quaternionic units, $e_i$, is that given by $e_i = -i\sigma_i$, where $\sigma_i$ are the 2 x 2 Pauli matrices. Pauli noted in his paper of 1927, where he introduced the matrices, that Jordan had pointed this out to him. Thus a quaternion can be represented by,

$$q = q_0 - iq_i\sigma_i = \begin{bmatrix} a & -b^* \\ b & a^* \end{bmatrix},$$

where,

$$a = q_0 - iq_3, \quad b = q_2 - iq_1.\quad (13)$$

In equation (12) the $^*$ represents complex conjugation. Thus a neat correspondence is obtained between quaternions and the SU(2) Lie group. In addition
the operator $U(\alpha)$ that rotates the 2-dimensional spinor representations of the rotation group by $\alpha$ about a direction $\hat{n}$ is given by [58]:

$$U(\alpha) = \exp(i \sigma \cdot \hat{n}) = \cos\left(\frac{\alpha}{2}\right) - i \sigma \cdot \hat{n} \sin\left(\frac{\alpha}{2}\right)$$

(14)

The similarity of this transformation with the Cayley-Rodrigues parametrization in equation (8) is immediately evident. In addition, equation (14) may readily be seen as a generalization of de Moivre’s theorem for complex numbers.

The second development we wish to mention is the association between division algebras and Lie groups. Through the work of Freudenthal, Rozenfeld and Tits, which may be found summarized in a review by Freudenthal [50], and in an application to supergravity by Günaydin et al. [51], it was realized that the four categories of semi-simple Lie groups, viz., orthogonal, unitary, symplectic and exceptional groups, were associated with the real numbers, complex numbers, quaternions and octonions via what is known as the “magic square.” Commenting on this rather remarkable result, Gürsey notes, that it associates the division algebras with “the very core of the classification of possible symmetries in nature” [23].

The third result is a beautiful relationship between the introduction of coordinates in affine and projective planes and the complex, quaternion, and octonion numbers [52]. With an affine plane associated with complex numbers the projective theorem of Pappus holds, whereas it does not for an affine plane associated with quaternionic structures. And while the theorem of Desargues holds for the latter plane, for the affine plane associated with octonionic structures neither the theorem of Desargues nor that of Pappus holds, although a more restricted form of the theorem of Desargues may be proved. This more restricted form was proved by Ruth Moufang in 1933.
4.2 Physical Applications

4.2.1 Quaternions and Spacetime Physics

The presence of four units in quaternions posed a problem of interpretation to Hamilton. Initially he had vaguely surmised that the vector part of the quaternion could be likened to a sort of “polarized intensity” while the scalar part to an “unpolarized energy.” Then in a letter to a friend in 1844 he wondered whether the vector part could represent the three space dimensions and the scalar part represents time. His latter view has been the way quaternions have been used to formulate special relativity, and their mathematical properties allow elegant expressions to be derived for all the expressions in special relativity.

Quaternions were first introduced into special relativity by Conway in 1911 and independently a year later by Silberstein. There has been a long tradition of using quaternions for special relativity and a review by Synge covers developments up until the 1960’s. Modern presentations have been given by Edmonds, Sachs, Gough and Abonyi et al. The use of quaternions in special relativity, however, is not entirely straightforward. Since the field of quaternions is a 4-dimensional Euclidean space, complex components for the quaternions are required for the 3 + 1 spacetime of special relativity. Quaternions of this nature were called biquaternions by Hamilton, and do not form a division algebra. Also there is a choice as to whether to express the scalar or the vector part of the quaternion in complex form. With the latter convention a spacetime point, \((ct, x_1, x_2, x_3)\), can be expressed as the quaternion

\[ x = ct + ix_1e_1. \]  

(15)

A Lorentz transformation of a boost, for example, of \(v\) in the \(x_1\) direction can be

\[ v = \gamma (ct - x_1e_1), \]

where \(\gamma = \frac{1}{\sqrt{1 - (v^2/c^2)}}\). This notation is similar to that used by Spinney and Proctor in their work on the subject.
written as \[54, 55, 59\]

\[\mathbf{x}' = \exp\left(\frac{i e_1 \theta}{2}\right) \mathbf{x} \exp\left(-\frac{i e_1 \theta}{2}\right), \quad \tanh \theta = \frac{v}{c}.\]  

(16)

Such a transformation leaves the norm \(\mathbf{x} \otimes \overline{\mathbf{x}} = (ct)^2 - x_i x_i\) invariant. Similar expressions may be formed for other spacetime quantities such as a four momentum and electromagnetic potentials, and electrodynamics can readily be given a quaternionic formulation \[61, 60\].

While an elegant reformulation of the equations of special relativity alone provides a motivation for the use of quaternions, various related avenues of research have emerged from this context. Rastall \[62\], Singh \[63\], and Sachs \[58\], for example, have shown there are certain advantages in representing field equations such as the Dirac equation and Maxwell equations in quaternionic form when a generalization is made to Riemannian space-time.

Various quaternionic formulations of Dirac’s relativistic equation have been considered the 1930’s onwards. Early presentations may be found in Conway’s work \[64\], and more recent presentations in the work of Edmonds \[57\], Gough \[59\], and Davies \[65\]. When written in this manner a doubling of the components of the wavefunction from four to eight occurs and the possible physical significance of these components has been a matter of speculation \[57, 59\]. Adler \[66\], for example, has exploited this feature to develop a novel form of QED which eliminates the need for a Dirac sea of negative energy electrons by combining both particle and antiparticle states within a single species of fermion. In addition, in an interesting paper Davies \[65\] has shown that when potentials are included in a quaternionic Dirac equation certain restrictions on their components are required which raise questions as to the observability of effects unique to a nonrelativistic quaternionic quantum mechanics.

Finally we note that the quaternionic formulation of spacetime theories has been extended to superluminal Lorentz transformations. Imaeda \[67, 68\] has
presented such a transformation for a boost in the $x_1$ direction in the form

$$x' = \pm i \exp(i \frac{e_1 \theta}{2}) x \exp(-i \frac{e_1 \theta}{2}) e_1, \quad \coth \theta = \frac{v}{c}, \quad (\frac{v}{c})^2 > 1 \quad (17)$$

Recently Teti has given an expression unifying both the subluminal and superluminal Lorentz transformations [69].

In these examples we can see how the extra structure of quaternions over complex and real numbers has enabled new perspectives through permitting different formalisms, and moreover, provided structures within which new physical theories can be considered.

### 4.2.2 Quaternionic Quantum Mechanics

In an important paper in 1936 Birkhoff and von Neumann [70] presented a propositional calculus for quantum mechanics, and noted that a concrete realization leads to a general result that a quantum mechanical system may be represented as a vector space over the real, complex and quaternionic fields. Their paper was the first to point out the possibility of a quaternionic formulation of quantum mechanics. Their result essentially means that the quantum mechanical superposition principle for probability amplitudes only determines the quantum mechanical probabilities to obey the “law of moduli” and thus to be one of the division algebras, and not necessary to be the algebra of complex numbers [71]. With a quaternionic extension the wavefunction may be given the form

$$\Psi = \Psi_0 + \Psi_i e_i, \quad (18)$$

where $\Psi_0$ and $\Psi_i$ are real. One can proceed to develop a quaternionic quantum mechanics (QQM) with states defined on a quaternionic Hilbert space. With such an extension the rays in the Hilbert space representing pure states are no longer one dimensional subspaces and the c-numbers no longer commute.
Studies on the application of quaternions in quantum theory go back to the 1950’s. The possibility of using quaternions as a basis for a field theory was considered by C. N. Yang in 1957. Since the phase in the complex algebra is associated with electromagnetism, Yang’s idea was to see if a phase in quaternionic algebra could be related to isotopic spin gauge fields that might then account for the existence of isotopic spin symmetry. While this hope was not fulfilled Yang noted in 1983 that he still believed the direction was a correct one.\footnote{Yang’s account of these attempts may be found in the introductory commentary to a collection of his papers \cite{Yang}. p. 22 -23.}

In the late 1950’s and early 1960’s several aspects of QQM were investigated in a series of foundational papers by Finkelstein et al. \cite{Finkelstein1, Finkelstein2, Finkelstein3, Finkelstein4}. Contemporary presentations of QQM may be found in the works of Adler \cite{Adler1, Adler2, Adler3, Adler4, Adler5}, Horwitz and Biedenharn \cite{Horwitz}, and Nash and Joshi \cite{Nash1, Nash2, Nash3, Nash4}.

QQM provides an excellent illustration of our principle as to how generalizations of certain mathematical structures can provide the avenues to explore new physical theories. QQM has many features which make it a far richer theory than complex quantum mechanics. It is not simply a matter of increasing the internal degree of freedom of one of the variables in the conventional complex theory, and defining many of the notions that correspond to the conventional theory has proved to be a difficult and interesting task. In particular, we mention the following issues which arise as unique concerns for QQM. To begin with, the proper generalization of the Schrodinger equation was by no means clear. Simply replacing the imaginary \(i\) of complex quantum theory in the Schrödinger equation proved not to provide the proper generalization. Rather, it was found the proper form for the Schrödinger equation is given by \cite{Adler1, Adler2},

\[
\frac{d\Psi}{dt} = -\overline{H}\Psi
\]  

where \(\overline{H}\) is a quaternion—anti-self-adjoint Hamiltonian. In addition, there is a
problem defining the tensor product of wavefunctions for composite systems due to the non-commutativity of wavefunctions such as in equation (18). A number of people have taken this as a reason to rule out QQM; however, a recent definition by Nash and Joshi [82] has provided a way to define such products, and moreover, to define them in a way that suggests how the effects of QQM may be hidden. Also, there has been the question as to whether phase transformations in the case of a quaternionic quantum field theory should be defined as having the form $\phi \rightarrow p\phi$, where $p$ is any unit quaternion, as Adler [72] indicates, or as $\phi \rightarrow p\phi p^{-1}$ as in the original papers of Finkelstein et al.. One recent study indicates there may be reasons for preferring the latter definition [84].

The relationship of QQM to complex quantum mechanics remains an interesting and unresolved issue. Could QQM apply to the realm of high energies, for example, or provide a theory for understanding preon dynamics while complex quantum mechanics only applies to presently observed particles? Or could QQM be a “cover” theory which applies to all particles, and reduce in some way to conventional quantum mechanics in realms where we have confirmation of the conventional theory? Related to these issues is the result of some interest that the correspondence principle of QQM does not entail a limit to some form of quaternionic classical mechanics but rather to a form of conventional quantum theory [72].

Finally, we should mention that one very significant result of the study of QQM was a formulation of a new form of gauge invariance by Finkelstein et al., which they have labeled as “Q-covariance” [76]. Given a quaternionic phase transformation of the form $\phi \rightarrow p\phi p^{-1}$, a statement that all of the physical laws are invariant to such a transformation leads to the introduction of a set of massive gauge bosons. There may be a connection between this manner of mass generation and the Higgs mechanism. If this proves to be true we may obtain new insights
into the profound problem of mass generation.

To achieve a clear resolution of some of these unsolved problems has both the potential to provide new physical theories, and at the same time to enable a better understanding of our present conventional quantum mechanics.

4.2.3 Some Recent Applications in Theories of Gravity

Complex numbers have played an important role in formulating various theories of gravitation. Spinors, for example, which are ordered pairs of complex numbers, provide powerful tools in exploring the structure of general relativity theory. In recent years various ways of extending the geometrical structure of general relativity have been considered such as in supergravity and Kaluza-Klein theories. Quaternions have also been used as a way to generalize the geometrical structure. For example, in standard general relativity theory the metric is a real bilinear form on a tangent space at each point in the spacetime manifold. Various extensions of the tangent bundle to other spaces have been considered such as to complex numbers and hypercomplex numbers. Mann [87] has recently considered a theory in which the tangent bundle is extended from a field of real numbers to one of quaternions. Mann’s approach introduces a non-Abelian framework into spacetime structure, but has the advantage of leaving features of conventional general relativity unchanged. In particular the spacetime manifold is real as well as quantities such as the invariant interval $ds^2$ defined on it.

Quaternionic structures have also been recently used to provide a possible framework in which to consider quantum theories of gravity. The work of Witten [88, 89, 90], for example, has shown the potential importance of topological considerations for the exploration of quantum field theories of relevance for general relativity. In addition, various elegant studies of 3-dimensional formulations of gravity as a gauge theory using a Chern-Simons action have been
given \([71, 72, 73, 88]\). The geometrical structures provided by quaternions may allow various 4-dimensional formulations to be obtained. Certainly quaternions have surfaced in considerations of \(N = 2\) supergravity, as the geometric structure of quaternionic manifolds is of interest to theories such as the non-linear sigma models that appear within supersymmetric theories \([74, 75]\).

The theoretical and experimental consequences of these studies are uncertain at the moment, however, we see how both the generality of the structures provided by quaternions, as well as the particular dimensions of their algebra are providing those structures of interest to the four dimensionality of spacetime.

### 4.2.4 Quaternions in Applied Physics

It is worth drawing attention to the rather remarkable way in which quaternions have emerged in recent decades in several applied areas outside of theoretical physics. While strictly outside the theme of this essay, we wish to mention some examples as their use in such areas will undoubtedly have an influence on their place within the physics of the future. It is often due to the use of certain mathematical structures in technological situations that they become part of the textbook tradition and the teaching of basic disciplines. One area of application arises from their excellent ability to represent rotations in three dimensional space, and the other through certain analytic properties of functions defined over quaternions. The contemporary practical applications of quaternions would have surprised some of the nineteenth century adversaries of quaternions. Heaviside in particular had noted that “it is practically certain that there is no chance whatever for Quaternions as a practical system of mathematics…” \([76]\), and Cayley stated that they seem “a very artificial method for treating such parts of the science of three-dimensional geometry” \([76]\).

In particular, the recent studies by Tweed et al. \([77, 78, 79]\), building on
pioneering work of Westheimer in 1957, have used quaternionic algebra to represent the intricate rotational motion in eyes movements. Both Westheimer and Tweed et al. note the advantages of computational efficiency as well as simplicity of expression when quaternions are used in the formulation of laws governing eye movements such as Listing’s Law. Quaternions have also been used for calculations needed in robotic control, computer graphics, and in determining spacecraft orientation. The shuttle’s flight software, for example, uses quaternions in its computation for guidance navigation and flight control. The advantages of the parameterization by quaternions (usually referred to as the “Euler parameters”) over other means such as the Euler angles include: i) speed of calculation; ii) avoidance of singularities; iii) providing a minimum set of parameters; iv) enabling other physical quantities such as angular momentum to be derived from the quaternionic parameterization in a particularly simple manner.

A second category of applications draws on the analytic properties of functions of quaternions that were investigated by Fueter in the 1930’s. A presentation of Fueter’s work in English may be found in a study by Deavours. Many of the results of complex analysis such as the Cauchy and Liouville Theorems generalize to quaternionic analysis and the powerful two dimensional results of complex analysis can be extended to three dimensions. In particular, this has recently been applied in a study by Davies et al. to the derivation of integral transforms of vector functions in three dimensions with an illustration of geophysical interest. It appears that quaternions form a natural co-ordinate system for vector integral transforms in three dimensions, and it may be surmised that using this feature of quaternions will provide a profitable approach to the study of integral transforms. The results are of immediate interest in areas such as geophysical exploration and remote sensing where integral transforms of fields in
three dimensions are used.

5 Conclusions

Our principle of the heuristic role of mathematical structures in physics specifies that those structures which are generalizations of structures currently part of successful physical theories will be the ones well suited for the development of new physical theories. Quaternions provide an illustration of some complexity, and in addition the status of the contemporary theories of which they are a part of is uncertain at the moment. Nevertheless several features emerge from this illustration that we would surmise occur whenever mathematical structures of this sort are used in physics.

First, the use of the generalized formalism provides structures from which new mathematical formalisms of use for physical theories may emerge. The manner in which vector analysis, with its separate cross and dot product, arose from the quaternionic product is one example of this occurring.

Second, often elegant ways of stating familiar results occur. The use of quaternions in any situations involving rotations in three or four dimensions, such as relativity theory expressed in Euclidean space, provide an example of how this may happen. In these cases there is cause to claim that the physical situation is revealed in a particularly clear manner by the formalism.

Third, attempts to use the formalism in new physical theories has potential to reveal more about the experiment and theoretical status of the theories which use the mathematical structures from which the generalization occurred. There are reasons to be optimistic that QQM will play this role. Even its failure to provide any viable physical theory has potential to illuminate the vital role complex numbers play in the theory.
Fourth, and indeed this is a rather important point, new physical theories can emerge using the generalized structures in a way that preserves many of the virtues of the theories associated with the previous mathematical structure. Again QQM may play a role such as this, and the various ways in which quaternions seem to be appearing in supergravity theories indicate a role for them of this nature.

Finally it is important to note that the particularity of the generalizations we are concerned with is one of the reasons they are productive in the search for new physics. The balance between each of Kitcher’s conditions for generalization ensures such a property. The generalized structures provide particular relationships which capture the particular features of nature. Mathematics plays an important role by limiting the possibilities for the physicist to consider.\(^\text{13}\) Quaternions generalize other mathematical structures in Kitcher’s sense, but have a particular four dimensional structure. Physicists who have used quaternions have noted this point. Tait, for example, noted in 1894, in response to an attack on quaternions due to their limited number of dimensions, that from a physical point of view this is not a defect, but “is to be regarded as the greatest possible recommendation.” For Tait it showed them to be particularly relevant to the “actual” world \(^{\text{114}}\). And 70 years later Rastall remarked that contrary to the spirit of certain rarefied mathematical approaches to spacetime theories, quaternions are useful to those “prepared to exploit the accident of having been born in space-time” \(^{\text{62}}\).

There is good reason then to see the active exploitation of certain mathematical generalizations as providing good guides for the physics of the future.

\(^{\text{13}}\)Zee, for example, stresses the value of this feature of mathematics, and notes that the limited number of Lie algebras is of extraordinary help in constructing GUTs \(^{\text{113}}\), p. 312.
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