How should spin-weighted spherical functions be defined?

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Spin-weighted spherical functions provide a useful tool for analyzing tensor-valued functions on the sphere. A tensor field can be decomposed into complex-valued functions by taking contractions with tangent vectors on the sphere and the normal to the sphere. These component functions are usually presented as functions on the sphere itself, but this requires an implicit choice of distinguished tangent vectors with which to contract. Thus, we may more accurately say that spin-weighted spherical functions are functions of both a point on the sphere and a choice of frame in the tangent space at that point. The distinction becomes extremely important when transforming the coordinates in which these functions are expressed, because the implicit choice of frame will also transform. Here, it is proposed that spin-weighted spherical functions should be treated as functions on the spin or rotation groups, which simultaneously tracks the point on the sphere and the choice of tangent frame by rotating elements of an orthonormal basis. In practice, the functions simply take a quaternion argument and produce a complex value. This approach more cleanly reflects the geometry involved, and allows for a more elegant description of the behavior of spin-weighted functions. In this form, the spin-weighted spherical harmonics have simple expressions as elements of the Wigner $\hat{D}$ representations, and transformations under rotation are simple. Two variants of the angular-momentum operator are defined directly in terms of the spin group; one is the standard angular-momentum operator $L$, while the other is shown to be related to the spin-raising operator $\delta$. Computer code is also included, providing an explicit implementation of the spin-weighted spherical harmonics in this form.

I. INTRODUCTION

Spin-weighted spherical functions form a primary technique in the study of waves radiating from bounded regions, and for observations of such radiation arriving at a point from all directions. The most important applications are found in gravitational-wave astronomy and in measurements of the cosmic microwave background. The basic motivation for these functions is quite simple: given any direction of the emission or observation, we would like the function to describe the magnitude of the wave, as well as any polarization information. This is achieved by using a complex number as the output of the function, where the wave magnitude is the complex amplitude, and the wave polarization is determined by the complex phase. However, an important subtlety arises. We need not only the propagation direction, but also a fiducial direction orthogonal to the propagation with respect to which the polarization may be measured. Thus, spin-weighted spherical functions (SWSFs) cannot be defined as functions on the sphere $S^2$ alone.

This statement may come as something of a surprise when compared to most of the literature on these functions.\(^1\)\(^-\)\(^8\) Traditional presentations of spin-weighted spherical functions write the functions in terms of spherical or stereographic coordinates for $S^2$. For example, spin-weighted spherical harmonics (SWSHs) generalize the standard scalar spherical harmonics, allowing for the decomposition of general (square-integrable) SWSFs into a sum of SWSHs. They are traditionally given by explicit formulas involving the usual polar and azimuthal angles ($\vartheta, \varphi$) or the complex stereographic coordinate $\zeta$. Such a presentation hides an implicit choice of frame in the choice of coordinate system. Indeed, it would be more correct to define spin-weighted spherical functions on coordinate systems for $S^2$, rather than on $S^2$ itself. As discussed below, one reference\(^9\) did actually define spin-weighted spherical functions in essentially this way, though doing so required mathematical tools that are not well known among astronomers or physicists. There is nothing inherently wrong with using coordinates—which are hardly to be avoided in any case—but this convoluted and unnatural approach causes many problems, both theoretical and practical. Probably the most disturbing is that in this guise SWSFs are generally multivalued or simply undefined at certain points on the sphere, depending on the coordinate system. Even away from those points, different coordinate systems will provide different canonical frames. In particular, a rotation of the coordinates leads to a rotation of the frame, which leads to a change in the value of the spin-weighted function at that point. That, in turn, leads to another prominent problem with this approach: in this lenient interpretation, spin-weighted spherical harmonics—unlike the more familiar scalar spherical harmonics—do not generally transform among themselves under rotation. That is, a SWSH in one coordinate system cannot be expressed as a finite linear combination of SWSHs in another coordinate system.

To avoid these problems, this paper defines SWSFs as functions from the spin group Spin(3) $\cong SU(2)$, which is best represented by quaternions. We will see that this space has a natural interpretation as the space of orthonormal frames on $S^2$, which is why it is the natural domain on which to define SWSFs. In practice, the quaternion achieves this by rotating the $z$ axis to a point on $S^2$, and rotating $x$ and $y$ into an orthonormal frame tangent at that point. Moreover, coordinate systems on $S^2$ and their associated canonical frames map naturally into Spin(3), in which case the value of our more general SWSHs agree precisely with their original definitions in terms of coordinate systems. Additionally, these SWSHs now form a representation of the group Spin(3), which means that they do transform among themselves. Finally, as a practical matter, the numerical implementation of SWSHs directly
in terms of Spin(3)—represented by quaternions—is just as fast and accurate as the implementation in terms of coordinates on $S^2$, if not more so.

A. Previous work

Newman and Penrose\cite{NewmanPenrose1963} introduced spin-weighted functions as a tool for the study of the asymptotic behavior of gravitational waves. They defined the differential operator $\delta$, which raises the spin weight of a function, and its adjoint $\bar{\delta}$ which lowers spin weight. One important feature of these operators is their explicit dependence on the spin weight of the functions on which they operate. Technically this means that there is a different operator labeled $\delta$ for functions of each spin weight. Newman and Penrose also used $\delta$ and $\bar{\delta}$ to define SWSHs as functions of coordinates on the sphere by raising and lowering the spin weights of scalar spherical harmonics.

Goldberg et al.\cite{GoldbergNewmanPenrose1969} further investigated the objects defined by Newman and Penrose, showing (among other things) that the formulas for SWSHs in spherical coordinates are identical to formulas for Wigner’s $\Sigma$ matrices for certain values of Euler angles—though no explanation was given for why this should hold. This extended the definition of SWSHs to allow for half-integer values of the spin weight. They also showed that $\delta$ can be expressed as something more like the traditional angular-momentum operator in terms of Euler angles, using the same definition regardless of the spin weight of the function on which it acts. This perspective is very close to the one proposed in the current paper. However, the authors remained bound by the idea that SWSHs should be defined on $S^2$, and by their devotion to Euler angles as a useful representation of rotations. As such, they merely provided a hint that a more general formulation is possible. This paper will show that it is in fact necessary from a mathematical perspective, and that it may be achieved in a simpler and more geometrically covariant fashion through the use of quaternions.

Though the use of spin-weighted functions gained currency in the analysis of gravitational radiation and—to a lesser extent—electromagnetic theory,\cite{PenroseRindler1984} related alternatives were used throughout the literature, in the form of symmetric trace-free tensors and various flavors of tensor spherical harmonics. Thorne\cite{Thorne1965} provided a useful overview and a translation between all these presentations. Dray\cite{Dray1986} later showed that essentially equivalent functions had been introduced separately as “monopole harmonics” to describe the motion of an electron in the field of a magnetic monopole. Penrose and Rindler\cite{PenroseRindler1986} showed that the SWSHs could be expressed in terms of contractions between tensor products of spinors, giving rise to SWSHs of half-integer spin weight—which is essentially an extension of the older symmetric trace-free tensor approach. In abstraction this approach avoids an explicit choice of basis, though such a choice is still required for any concrete application, as discussed in Sec. I.B.

In a substantial departure from techniques found in previous literature, Eastwood and Tod\cite{EastwoodTod2014} were apparently the first to define spin-weighted functions “on the sphere” in a mathematically rigorous form. They (somewhat generously) reinterpreted earlier work as defining spin-weighted functions as pairs of functions defined on complementary coordinate patches of the sphere. But they went on to generalize this by introducing their own definition in terms of a “sheaf of germs of functions”. This is not common language in the physics literature, and it will be argued below that there is a simpler approach, so the reader who is not interested in the details of this formulation may wish to skip the remainder of this paragraph, and perhaps the next. In the treatment by Eastwood and Tod, each function of spin weight $s$ is defined on $\mathbb{CP}^1$, the projective reduction of the complex space $\mathbb{C}^2 \setminus \{(0,0)\}$. The germs are defined by the local condition that at any point $\pi \in \mathbb{CP}^1$ a function $s f$ having spin weight $s$ must obey

$$s f(\lambda \pi) = \left( \frac{\lambda}{\bar{\lambda}} \right)^s s f(\pi) \quad (1)$$

for any nonzero $\lambda \in \mathbb{C}$. Only the phase of $\lambda$ is relevant on the right-hand side, so this property essentially describes the behavior of $s f$ under rotation of the coordinates about $\pi$—which is closely related to the standard motivation for spin-weighted functions, as described below. While the germs enforce the spin-weight property locally, the sheaf represents the collection of these germs at different points. In particular, the sheaf structure ensures that the functions are compatible on the intersections of any local coordinate charts. Basically, this generalizes the definition of spin-weighted functions as pairs of functions on complementary coordinate patches to deal with not just two patches, but with arbitrary collections of coordinate patches.

To obtain values for any SWSF, we must choose coordinates of $\mathbb{CP}^1$. It is well known that this is impossible over the entire topological sphere $S^2$; at least one point in the sphere cannot be covered by a nonsingular coordinate patch. This prescription can therefore only describe the value of SWSFs over the entire sphere if they go to zero at that particular point, or if multiple coordinate patches are used. Thus, we see that the incorporation of sheaves is not mere superfluous formalism, but is actually necessary to a consistent formulation of SWSFs as being—in any sense—functions “on the sphere”. It should be noted that, although we can identify $\mathbb{CP}^1$ topologically with $S^2$, spin-weighted functions still cannot simply be considered functions on $S^2$; there is additional complex algebraic structure needed to define them, which is present in $\mathbb{CP}^1$ but not in $S^2$. Specifically, Eq. (1) requires complex conjugation and multiplication, while the mapping from $\mathbb{CP}^1$ to $S^2$ requires a choice of basis. These allow us to choose preferred directions on $S^2$ using, for example, the real part of the coordinates. But these are additional structures that are not present on $S^2$ alone.

The work of Eastwood and Tod encompasses and supersedes previous work, propelled by their insightful and rigorous approach. They step back to look at the underlying mathematical structures needed to define spin-weighted functions, and do so in a way
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that is—abstractly, at least—-independent of any particular choice of coordinates on the sphere. From a purely mathematical perspective, this approach is entirely satisfactory. However, the very simple geometric motivation for these functions is hidden behind the complicated and subtle constructions needed to adequately present spin-weighted spherical functions as functions on \( \mathbb{C}P^1 \). By leaving \( \mathbb{C}P^1 \) and \( S^2 \) aside, we will find a simpler, more direct, and geometrically intuitive approach.

In this approach, we avoid the complicated language of sheaves because the functions can be defined globally, so that the sheaf structure is essentially trivial. This is done by choosing a different domain on which to define SWSFs. The approach taken in the present paper was first presented by the author in the open-source software package SphericalFunctions.\(^{11}\) It consists of defining SWSFs as functions from the spin group Spin(3) \( \cong \text{SU}(2) \) to the spinor algebra generated by a two-dimensional vector subspace. Though these terms may sound unfamiliar, essentially we will just have functions from the group of unit quaternions\(^{12}\) to \( \mathbb{C} \)—though we will also find surprisingly simple and helpful geometric interpretations. This approach was developed, though not explored in depth, in previous papers.\(^{13,14}\) A similar approach was described in depth by Straumann,\(^{15}\) who chose to define SWSHs as functions from SO(3) to a two-dimensional vector space. SO(3) maps to \( S^2 \) by rotating the z axis to any point on the sphere (as discussed further in Sec. III C). The vector space in which the SWSHs take their values is the tangent space to the sphere at that point. One fairly minor fault in Straumann’s approach is that it does not account for functions of half-integer spin weight because of the use of SO(3) in place of Spin(3). However, Straumann’s approach also requires relatively esoteric methods from differential geometry and Lie theory. Using quaternions, we will be able to remain close to the geometric origins of SWSFs, especially when defining the differential operators.

B. Tensor-valued spherical functions and the limits of abstraction

Although complex-valued SWSHs dominate the literature in observational astronomy, another description of tensor fields also frequently provides important benefits: tensor-valued spherical harmonics, which are functions from the sphere \( S^2 \), taking values in complex tensors over the tangent space. The latter may be the tangent space intrinsic to the sphere at that point, or—more frequently—may be “tangent” to the usual three-dimensional space in which the sphere is embedded so that the normal may be included. While a full review\(^4\) of tensor spherical harmonics is beyond the scope of this paper, a brief discussion is in order so that we may clarify their relation to the present work. In particular we will see that tensor spherical harmonics are naturally suited to abstract formal calculations, and as such they do not require a choice of frame tangent to \( S^2 \) when treated abstractly, but are fundamentally equivalent to SWSHs in applications.

We can apply three main types of abstraction in analysis of tensor spherical harmonics. First, we may construct tensor spherical harmonics as tensor fields starting with the metric, the normal vector, and the Levi-Civita symbol, and tensor products thereof. Starting from these basic components, the field is given angular dependence either by taking a further tensor product with covariant derivatives of a scalar spherical harmonic, or the scalar product is taken with a scalar spherical harmonic.\(^{4,7}\) The tensorial part of this formulation is invariant in the standard way.\(^{16}\) Abstractly, these tensor spherical harmonics have various algebraic, combinatorial, and differential properties that are true independent of any frame that may be chosen to express components of those tensors. This means that various manipulations can be carried out very efficiently in abstraction. Relationships between fields may be found using the abstract tensor objects, and invariant scalar fields may even be defined by contractions of two or more tensor fields. In a similar way, we can abstractly discuss the dependence of tensor and scalar fields on location. We posit the existence of some point \( p \), which we suppose has a geometric meaning independent of any coordinate system that may be used to describe that point. We might discuss the effect of a transformation that changes the point referred to by \( p \), or the differential behavior of the fields as we vary the position at which they are evaluated. Finally, for many purposes the scalar spherical harmonics need not be defined concretely; we may simply stipulate that they are continuous, or differentiable at some level, or that they form a complete basis for some space of functions, or that they transform in certain ways under rotations. Their particular functional dependence is—in many cases—irrelevant if we can assume certain abstract properties. In each of these ways, the abstract methods of mathematics can be applied to understand deep and general properties of tensor spherical functions.

As undeniably useful as abstract manipulations are for general theoretical investigations, using tensor spherical harmonics in practice means abandoning the abstract for the concrete, because a measurement produces concrete values for the field, and scientific models frequently need to predict concrete values. First, and most simply, we need to determine the point at which the field is to be measured. Then we need to define the scalar spherical harmonics as functions of that point—which will naturally depend on how we specify the points. Finally, we need to express the tensor in terms of its components with respect to a specific basis. All three of these tasks are typically accomplished using arbitrary coordinates, and some more-or-less natural vector basis derived from those coordinates. Even when a tensor field is contracted with a tensor spherical harmonic to form a scalar mode weight, that scalar ultimately depends on the particular functional form chosen for the scalar spherical harmonics, and will transform under rotations or other transformations of the coordinate system. Spin-weighted spherical harmonics can be expressed as contractions between elements of such vector bases and tensor spherical harmonics, just as tensor spherical harmonics may be expressed as scalar multiples of spin-weighted spherical harmonics with various combinations of the vector-basis elements.\(^3\)

Thus, we see that tensor and spin-weighted spherical harmonics are precisely equivalent whenever concrete formulations are used. And naturally, observations—as well as many types of calculations—cannot be performed based on only the abstract...
properties of the fields and harmonics. We will see in Sec. V how scalar spherical harmonics and \textit{mode weights} of SWSHs transform among themselves under rotations, which avoids many of the concrete elements mentioned above—though not all. On the other hand, there is no known closed-form expression describing transformations of the mode weights or scalar spherical harmonics under the Lorentz group. Instead, values of the field may be computed explicitly at particular points and possibly used for decomposition into mode weights.\textsuperscript{14} This construction, of course, requires various concrete elements, which can be manipulated much more easily when spin-weighted functions are defined on the spin group.

C. Summary of this paper

We begin by reviewing spin-weighted functions and their original geometric motivation in Sec. II. In particular, we will see that SWSFs require a selection of an orthonormal frame for the tangent space to the sphere—which will show very explicitly why it is impossible to define spin-weighted functions as functions solely on $S^2$. However, this will also suggest how SWSFs should be defined. In Sec. III, careful topological arguments will show how the geometry behind the spin-weighted functions is appropriately identified by the Hopf bundle. The Hopf bundle is essentially a mapping from Spin(3) to the sphere $S^2$, though it carries along extra structure relating to the tangent frame of the sphere—it is essentially the orthonormal frame bundle of $S^2$. Thus, rather than keeping track of the basis vectors in the frame, we can simply keep track of the rotation required to take some reference frame onto any other frame. This will explain why Spin(3) is the natural domain on which to define SWSFs.

However, the codomain (the space into which SWSFs map) is not uniquely defined by these arguments. In Sec. IV, we will see that several interpretations are possible and equally valid. One interpretation of the codomain for SWSFs of integer weight is the space of vectors in the $\mathbf{x}$-$\mathbf{y}$ plane. For SWSFs of more general (possibly half-integer) weight, the equivalent codomain would be the algebra of spinors generated by vectors in that plane. We will see that the $\mathbf{x}$-$\mathbf{y}$ plane is a convenient choice, but any two-dimensional Euclidean vector space will do—in particular, the plane tangent to $S^2$ at the given point holds obvious significance. And of course, any such structure is generically isomorphic to the complex numbers $\mathbb{C}$, which is the most common codomain by which SWSFs are defined in the literature. However, one guiding criterion may be the relationship to the polarization in the tangent space, as mentioned above—which would seem to indicate that the use of $\mathbb{C}$ ignores that important piece of geometry.

It turns out that Wigner’s $\Xi$ matrices provide a particularly useful basis for (square-integrable) complex-valued functions on Spin(3), which explains why Goldberg et al.\textsuperscript{2} found the correspondence noted above. These will be derived in Sec. V using a geometric approach. Using the quaternionic presentation of Spin(3), this allows us to express the $\Xi$ matrices directly in terms of a quaternion argument. In its simplest form, this expression is essentially the same as the one found by Wigner:\textsuperscript{17}

\begin{equation}
\Xi^{(\ell)}_{m',m}(\mathbf{R}) = \sqrt{(\ell + m)!(\ell - m)!/(\ell + m')!(\ell - m')!} \sum_{\rho} \left[\begin{array}{c}
\ell + m' \\
\rho \\
\ell - m'
\end{array}\right] \left[\begin{array}{c}
\ell - m' \\
\rho \\
\ell - m
\end{array}\right] (-1)^{\rho} R^\rho_{\ell} R^\rho_{\ell'} R^{\rho - m - m'} R^\rho_{m'} R^\rho_{m},
\end{equation}

where $R_\rho$ and $R_\rho'$ are geometric projections of the quaternion $\mathbf{R}$ into “symmetric” and “antisymmetric” components, and are simply complex combinations of the components of the quaternion. However, by paying particular attention to special cases where this expression encounters numerical difficulties, we can find a more robust formula, given in Eq. (35). Moreover, an efficient algorithm for evaluating that formula will be described, which avoids explicit computation of the binomial factors and avoids most of the delicate cancellations of terms in the sum.

The group structure of Spin(3) allows us to define two types of differential operators, as discussed in Sec. VI. One will turn out to be the standard angular momentum operator $\mathbf{L}$, while the other will turn out to be the operator $\mathbf{K}$ introduced by Goldberg et al.\textsuperscript{2} The lowering and raising operators associated to $\mathbf{K}$ are precisely the spin-raising operator $\delta$ and the spin-lowering operator $\delta$ first introduced by Newman and Penrose. This, finally, allows us to define spin-weighted spherical functions in general as eigenfunctions, according to Eq. (48), of the component of $\mathbf{K}$ selected by the choice of codomain.

The paper concludes in Sec. VII by summarizing what has been found, and returning to the physical problem of describing radiation. Appendix A describes an algorithm to improve the direct evaluation of the Wigner $\Xi$ (hence also SWSH) functions, which improves the speed and accuracy for which they can be evaluated for $\ell \leq 12$. Appendix B is also included to provide a discussion of various parametrizations of Spin(3) and $S^2$, and their various strengths and weaknesses. It will be suggested that the usual unit quaternions constitute the best presentation of Spin(3), though it also turns out that the standard spherical coordinates $(\theta, \varphi)$ are entirely adequate for describing values of spin-weighted functions on $S^2$ despite the coordinate singularities—as long as no transformations are required.

II. REVIEW OF SPIN-WEIGHTED FUNCTIONS

Here, we briefly review SWSFs and SWSHs—taking a general geometric approach, without getting into details of the presentations in earlier work, but emphasizing the features that will be most important to this paper. To begin, we simply assume a standard three-dimensional vector space with the usual Euclidean norm. Consider some direction represented by the unit vector $\mathbf{e}$.
vector \( n \). The space of all such directions is—naturally—the sphere \( S^2 \), which is why these functions are sometimes described as if they were functions on \( S^2 \). Next, we construct an orthonormal frame \( (a, b, n) \). The orientation of this frame is fixed by insisting that it be a right-handed triple. The attitude of the frame, however, is not determined. Given only the direction \( n \), there is no unique prescription for \( a \) and \( b \); they may be rotated in their own plane without changing the required properties.

At this point, it is customary to introduce the complex vector

\[
m := \frac{a + i b}{\sqrt{2}}.
\]

This complexification of the vector space is merely a convenient bookkeeping device with no deeper significance, but will simplify many manipulations below. If we have another frame \( (a', b', n) \) such that our original frame is given by a rotation of this new frame through an angle \( \gamma \) about \( n \), we also obtain a new complex vector \( m' = e^{i\gamma} m \). A function \( s \) defined on this frame is said to be of spin weight \( s \) if, given this transformation of the frame vectors, the value of the function transforms as

\[
s_f(m', n) = e^{is\gamma} s_f(m, n).
\]

Clearly, if the spin-weighted function is defined only in terms of these vector arguments, a rotation through \( \gamma = 2\pi \) must return the function to its original value, which means that \( s \) must be an integer. We will also see that it is possible to define spin-weighted functions with a spinorial character, so \( s \) will also be able to take half-integer values.

It is easy to find some very simple examples of functions of spin weight \(-1, 0, 1\) respectively:

\[
\begin{align*}
-1f(m, n) &= z \cdot \bar{m}, \\
0f(m, n) &= z \cdot n, \\
1f(m, n) &= z \cdot m.
\end{align*}
\]

Here, \( z \) is just the usual unit vector in the \( z \) direction. Though \( z \) is obviously independent of \( m \) and \( n \), these functions are not constant on the sphere because of the position dependence of \( m \) and \( n \). Moreover, any vector could be used in place of \( z \), so that for each value of \( s \) we have a three-dimensional complex vector space of functions. In fact, these spaces are exactly the spaces of spin-weighted spherical harmonics \( sY_{\ell,m} \) with \( \ell = 1 \). More generally, spin-weighted functions can be constructed by replacing \( z \) in Eqs. (5) with some other symmetric and trace-free complex tensor of rank \( \ell \). This must then be contracted with a corresponding tensor product of the \( m \), \( \bar{m} \), and \( n \) basis elements, which replaces the factors on the right-hand sides of Eq. (5). The set of all such tensors of rank \( \ell \) forms a complex vector space of dimension \( 2\ell + 1 \), which transforms within itself under rotation. The spin-weighted spherical harmonics \( sY_{\ell,m} \) form a standard basis for this space; an arbitrary square-integrable spin-weighted function can be expressed as a sum of these harmonics for various \( \ell \) values. As usual, these functions are necessarily 0 for \( |m| > \ell \). For similar reasons, SWSHs with \( |s| > \ell \) must also be 0.

But if we are concerned with the value of a function in more than one direction, we need to allow for more general transformations than the one described around Eq. (4). In particular, a rigid rotation of the sphere will only be about \( n \) for two directions. More generally, the transformed frame is \( (a', b', n') \). We still have a transformation law of the form

\[
s_f(m', n') = e^{is\gamma'} s_f(m, n),
\]

but now \( \gamma' \) is some complicated function of \( (m', n') \) and the rotation used to implement the transformation. This is seen most dramatically in the transformation law for SWSHs under rotation in the standard presentation. As we will show below, that law is

\[
s_f Y_{\ell,m}(\theta, \varphi) = \sum_{m'} s_f Y_{\ell,m'}(\theta', \varphi') \tilde{s}_{m'm}^{(\ell)}(R) e^{is\gamma'(\theta', \varphi', R)}.
\]

We will compute the functional form of \( \gamma' \) in Sec. V A, but the important point for now is that it is the nontrivial—and in fact discontinuous. Thus, it is incorrect whenever \( s \neq 0 \) to say that the SWSHs transform among themselves, or that they transform under a representation of the rotation group. The case of \( s = 0 \) corresponds to the usual scalar spherical harmonics, and we are familiar with the fact that their transformation properties under rotation are very important to their practical application, so we need to find a suitable setting in which the spin-weighted harmonics with \( s \neq 0 \) have comparable features. More generally, to describe SWSFs properly, we need an adequate presentation of the tangent frame, given a direction \( n \). This is the subject of the following section.

### III. SPECIFYING THE TANGENT FRAME AND THE DOMAIN OF SWSFS

We saw in Sec. II that the value of a spin-weighted function is formed at a given point by contractions between a tensor and the basis elements of some frame—in particular a frame of the vector space tangent to the sphere. But those basis elements...
can transform among themselves, which can change the value of the spin-weighted function. Therefore, to find the value of a
spin-weighted function, we need to specify not only a point on the sphere $S^2$, but also an orthonormal frame at that point. In this
section, we will see how to properly describe the orthonormal frame at each point.

It is not hard to see that the set of orthonormal tangent frames at a given point (assuming a certain orientation) is topologically a
circle $S^1$. The directions described above by the pair of orthogonal unit vectors $a$ and $b$ can only rotate in their own plane, so the
space of all right-handed orthonormal frames defined by $n$ is precisely the set of all directions of $a$ in that plane, which is just
the circle $S^1$. Spin-weighted functions must respect this topology in the sense described by Eq. (4): they must be periodic under
rotations of the tangent space. A similar restriction arises from the requirement that spin-weighted functions must be continuous
as $n$ moves around the sphere. To understand this more subtle restriction, we need to be more precise in our definitions. In doing
so, we will discover the appropriate domain of definition for spin-weighted spherical harmonics.

A. The fiber bundle and the attitude map

We first need a way to relate each possible point in the sphere to each possible choice of attitude of the tangent frame. This isnaturally given by the concept of the fiber bundle. We define our base space to be $S^2$ and our fiber space to be $S^1$. Then the fiber
bundle is defined as some “total” or “entire” space $E$ along with a projection map $p : E \rightarrow S^2$. This map is required to have the
property that for any point in the base space $b \in S^2$, the set of all points in the entire space $E$ that map to $b$ (the “preimage” of $b$),
or simply “fiber” over $b$ is topologically the same as our fiber space:

$$p^{-1}(b) = \{ e \in E \ | \ p(e) = b \} \equiv S^1.$$  

By defining our spin-weighted function on this fiber bundle, we can ensure that its value returns to itself under rotation in the fiber
space and—more importantly—under rotation of the point in $S^2$.

However, there are at least two distinct possibilities for the space $E$. To choose between them, we need to make the relationship
between $S^1$ and the tangent space more explicit. We define an “attitude map” taking a point $e \in E$ to an element of the unit tangent
space of the sphere at the corresponding point:

$$a : E \rightarrow UT_{p(e)}(S^2),$$  

so that

$$a(e) \in UT_{p(e)}(S^2).$$

We require that this function be continuous. At this point, we do not need to know the actual form of this function; let us simply
assume that such a function exists. We need this assumption because if, as we will claim, this fiber space constitutes the correct
domain on which to define SWSFs, we must have some compatible way to construct the tangent frame $(a, b, n)$ used in the
definition of SWSFs in Sec. II.

The most obvious candidate for the bundle is the trivial bundle with $E = S^2 \times S^1$, where the projection map $p : S^2 \times S^1 \rightarrow S^2$

is the simplest one:

$$p(b, f) = b.$$  

This fulfills the requirements of being a fiber bundle. The problem is that in this case, we can easily find a “global section”, which
is a continuous map $s : S^2 \rightarrow E$ such that the composition of the projection map and the section map $p \circ s$ is just the identity
function on all of $S^2$. For example, we can simply choose some point $f \in S^1$ and define the section map as $s(b) = (b, f)$. This is
well defined for all $b \in S^2$, it is trivially continuous, and we have $p(s(b)) = b$. But now, if we assume the existence of an attitude
map $a$, we can construct a continuous nonvanishing vector field over the sphere defined by the function

$$a \circ s : S^2 \rightarrow UT_a(S^2).$$

This violates the Hairy-Ball Theorem, which says that no such vector field can exist. Since we have exhibited the map $s$, this
contradiction tells us that our assumption about the existence of an attitude map $a$ is wrong. No such attitude map can exist on
the bundle with $E = S^2 \times S^1$, so this bundle is not an adequate model for the space on which spin-weighted functions should be
defined.

B. The Hopf bundle and the spin group

We have shown that the naive choice of the trivial fiber bundle is not sufficient. Fortunately, there is another well known
example of an $S^1$ bundle over $S^2$: the Hopf bundle. The total space of this bundle is $E = S^3$. Not only is this the appropriate
representation, allowing us to directly define simple functions for both the bundle projection map and the attitude map, it will also give us a clear geometric picture of the relationships between the spaces.\(^\text{28}\)

We begin with the traditional presentation of the Hopf map, by expressing the various spheres in terms of their standard embeddings into Cartesian space of one additional dimension: \(S^1 \subset \mathbb{R}^2\), and so on. Now, if a point on \(S^3 \subset \mathbb{R}^4\) has Cartesian coordinates \((w, x, y, z)\), the Hopf map \(h : S^3 \to S^2\) is defined by\(^\text{29}\)

\[
h(w, x, y, z) = (2wy + 2xz, 2yz - 2wx, w^2 - x^2 - y^2 + z^2),
\]

where the right-hand side gives the point in Cartesian coordinates of \(\mathbb{R}^3\). This is the projection map of the fiber bundle. Some straightforward but wholly unenlightening algebra can be used\(^\text{30}\) to show directly that the preimage is indeed homeomorphic to \(S^1\); we will see this in a more elegant and enlightening way below.

More interestingly, we can treat points in \(S^3 \subset \mathbb{R}^4\) as unit quaternions, and points in \(S^2 \subset \mathbb{R}^3\) as unit vectors. The unit quaternions form a group: the spin group \(\text{Spin}(3)\). A unit quaternion \(\mathbf{R}\) acts by conjugation on the unit vector \(\mathbf{z}\) in \(\mathbb{R}^3\), using quaternion multiplication:

\[
\mathbf{v} = \mathbf{R} \mathbf{z} \mathbf{R}^{-1}.
\]

Here and below, we implicitly map between vectors and pure-vector quaternions where needed by adding or removing a scalar component 0. If \(\mathbf{R}\) has components \((w, x, y, z)\), then \(\mathbf{v}\) has components given by Eq. (12). That is, rotation of \(\mathbf{z}\) by \(\mathbf{R}\) is another expression of the Hopf map:

\[
h(\mathbf{R}) = \mathbf{R} \mathbf{z} \mathbf{R}^{-1}.
\]

This quaternionic presentation of the Hopf map has other nice features: it allows us to explicitly calculate the fiber of any point, and it is very closely related to the attitude map.

To calculate the fibers, we first find a single element of the fiber over each point. For each \(\mathbf{v} \neq -\mathbf{z}\), we map

\[
\mathbf{v} \mapsto \frac{1 - \mathbf{v} \mathbf{z}}{\sqrt{2 + 2 \mathbf{v} \cdot \mathbf{z}}},
\]

and for the remaining point we arbitrarily choose

\[
-\mathbf{z} \mapsto e^{\pi \mathbf{z}/2}.
\]

It is not hard to show that the results are unit quaternions, and correctly transform \(\mathbf{z}\) into the desired vector in each case. That is to say that they are indeed elements of the fiber over the respective points. Now given a single point in the fiber, we can find all other points as follows.

Assuming \(\mathbf{R}\) and \(\mathbf{R}'\) represent two unit quaternions in the fiber over a point, we know by definition that they map to the same point on the sphere,

\[
\mathbf{R} \mathbf{z} \mathbf{R}^{-1} = \mathbf{R}' \mathbf{z} \mathbf{R}'^{-1}.
\]

Intuitively, we would expect that the rotations represented by these quaternions can only differ by an initial rotation about \(\mathbf{z}\). To see this more rigorously, we define \(\mathbf{S} := \mathbf{R}^{-1} \mathbf{R}'\) and rearrange Eq. (16) to show that \(\mathbf{S} \mathbf{z} = \mathbf{z} \mathbf{S}\). That is, \(\mathbf{S}\) commutes with \(\mathbf{z}\). The only quaternions with this property are linear combinations of scalars and elements proportional to \(\mathbf{z}\). Furthermore, \(\mathbf{S}\) has unit norm, as we can see from its definition. All unit quaternions can be written in the form \(e^{i\mathbf{u}/2} = \cos \frac{\theta}{2} + \mathbf{u} \sin \frac{\theta}{2}\), for some unit vector \(\mathbf{u}\) and some scalar \(\theta\). Applied to this situation, that means \(\mathbf{S}\) must be of the form \(\mathbf{S} = e^{\gamma \mathbf{z}/2}\) for some real number \(\gamma\); equivalently, we must have \(\mathbf{R}' = \mathbf{R} e^{\gamma \mathbf{z}/2}\). Obviously the exponential is periodic in \(\gamma\) with period \(4\pi\) (though the action of this quaternion rotating any vector has period \(2\pi\)). Meanwhile, \(\mathbf{R}\) can be any unit quaternion taking \(\mathbf{z}\) onto the point of \(S^2\) in question. Thus, we can calculate the fiber of any point on the sphere. For \(\mathbf{v} \neq -\mathbf{z}\), we have

\[
h^{-1}(\mathbf{v}) = \left\{ \frac{1 - \mathbf{v} \mathbf{z}}{\sqrt{2 + 2 \mathbf{v} \cdot \mathbf{z}}} e^{\gamma \mathbf{z}/2} \middle| \gamma \in \mathbb{R} \right\},
\]

and we have

\[
h^{-1}(-\mathbf{z}) = \left\{ e^{\pi \mathbf{z}/2} e^{\gamma \mathbf{z}/2} \middle| \gamma \in \mathbb{R} \right\}.
\]

By the periodicity in \(\gamma\), we see that each such fiber is indeed homeomorphic to \(S^1\).
Spin-weighted spherical functions

Now, because each fiber is topologically $S^1$, it can be used to represent a unique choice of direction in the tangent space. However, it remains to be seen whether or not this can be done in a continuous way on the entire space $E = S^3$. That is, we need to show that there exists an attitude map $a$ as in Eqs. (9). We define

$$a(R) = R \times R^{-1}. \tag{18}$$

The resulting vector is orthogonal to $v = R z R^{-1}$, and thus can be considered to be an element of the tangent space to the sphere at that point. The right-hand side of Eq. (18) is a rational polynomial in the components of $R$, and so is continuous everywhere the denominator does not go to 0, which is everywhere $R \neq 0$. Of course, we assumed that $R$ must have unit norm, so this condition is always satisfied, which means that we have found an acceptable attitude map.\(^{31}\)

We can evaluate this map on any element of the same fiber to find

$$a(R e^{\gamma z/2}) = R e^{\gamma z/2} x e^{-\gamma z/2} R^{-1}, \tag{19a}$$

$$= e^{\gamma x/2} R x R^{-1} e^{-\gamma x/2}, \tag{19b}$$

$$= e^{\gamma x/2} a(R) e^{-\gamma x/2}. \tag{19c}$$

The final form of this expression shows that it is just the rotation through an angle $\gamma$ about $v$—in other words, it is a rotation of the tangent space as we would expect. Having exhibited the existence of the map $a$, the Hairy-Ball Theorem now tells us that there does not exist any global section $s$ of the Hopf bundle. The map given by Eqs. (15) only constitutes a local section because it is discontinuous at $-z$. Thus, we avoid the contradiction found above for $E = S^2 \times S^1$.

The unit quaternions provided us with a simple realization of both the Hopf bundle and the attitude map, as well as a clear geometric picture of the relationship between the various spaces. This suggests that the group of unit quaternions—the spin group $Spin(3)$—is, in some fundamental way, the appropriate domain on which to define spin-weighted spherical functions. There is, however, a minor subtlety in the attitude map, which might suggest a slightly different domain, as we see next.

C. Degree of the attitude map and the domain of spin-weighted spherical functions

In the above, an important feature of the projection and attitude maps can be seen, but was not discussed explicitly. Both $h$ and $a$ [Eqs. (14) and (18)] involve $R$ quadratically, meaning that $R$ and $-R$ map to the same elements under both maps. Since we have constructed these maps as rotations of vectors, the interpretation is clear: the $Spin(3)$ group we have used is implicitly projected down to $SO(3)$, and the former is a double cover of the latter. We can also view this from another perspective. Restricting attention to a single fiber, the attitude map $a$ takes the fiber $S^1$ to the space of unit tangent vectors, which is also homeomorphic to $S^1$. But this map has degree 2. That is, the tangent vector $a(R e^{\gamma z/2})$ rotates twice as $\gamma$ goes from 0 to $4\pi$, even though these different values of $\gamma$ all correspond to distinct quaternions on the fiber before returning back to the starting point at $\gamma = 4\pi$. The reason for this strange behavior is that we are considering tangent vectors manipulated by spinors; vectors have spin 1, whereas spinors have spin 1/2.

We can, if we wish, remove this strange feature by defining another fiber bundle with this redundancy removed. Here, the entire space is just the projective sphere $\mathbb{RP}^3$, which is equivalent to the sphere $S^3$ with antipodal points identified. This is naturally the topology of $SO(3)$, so we can identify each point in $\mathbb{RP}^3$ with an operator in $SO(3)$. Then, we can again form a projection map $p : \mathbb{RP}^3 \to S^2$ by taking $p(R) = R(z)$, which is just the vector $z$ rotated by $R \in SO(3)$. Similarly, we can define the attitude map as $a(R) = R(x)$. This is nearly the same construction as above,\(^{32}\) except that this attitude map has degree 1.

However, this projective construction is somewhat complicated. And there is no particular reason to avoid the original formulation in terms of $Spin(3)$; we can still use it to construct functions of integer spin weight in a natural way, even with this small amount of redundancy. More importantly, we can also use $Spin(3)$ to construct functions of half-integer spin weight—for which we cannot use $SO(3)$. Finally, as a simple practical matter, parametrizations of $SO(3)$ either are just parametrizations of $Spin(3)$ with this redundancy present, or can be extended trivially to parametrizations of $Spin(3)$—as will be discussed further in Appendix B. Taken together, these arguments indicate that there is no good reason to restrict the domain to $SO(3)$, and every reason to use $Spin(3)$ as the domain instead.

IV. THE CODOMAIN OF SWSFS

Now, having settled on the appropriate domain for SWSFs, we need to understand the codomain in which these functions will take values. Traditional presentations\(^{1,2,6,9}\) chose the complex numbers $\mathbb{C}$ as the codomain. It should be noted that the spinor space over any two-dimensional vector space with Euclidean norm is—algebraically speaking—identical to the complex numbers,\(^{33}\) but the geometric interpretation of this codomain is not clear. An intuitively obvious choice would be the vector space of the $a \cdot b$
plane, where
\[
\begin{align*}
a &:= R x R^{-1}, \\
b &:= R y R^{-1}.
\end{align*}
\] (20a) (20b)

If we think of the set of all directions \( n := R z R^{-1} \) as comprising a sphere \( S^2 \) embedded in \( \mathbb{R}^3 \), the \( a \cdot b \) plane is just the tangent plane at \( n \). This would be in line with our original motivation for SWSFs as representing the component of some radiated or received wave. This interpretation is technically slightly complicated because the codomain in this case would be the spinor space of the entire three-dimensional vector space, but the function on \( R \) would only take values in the spinor subalgebra corresponding to the plane spanned by the vectors of Eqs. (20).

Alternatively, \( C \) could correspond to the spinor space of the \( x \cdot y \) plane, independent of the argument of the function. This is a somewhat tidier choice, as the codomain is "minimal" in some sense. Geometrically, the \( x \cdot y \) plane can be rotated onto the \( a \cdot b \) plane by \( R \). Algebraically, the spinor is rotated by conjugation by \( R \), just as the vectors are in Eqs. (20). So we could use the same interpretation of the spinors as describing the \( a \cdot b \) plane, even though the actual function values are in the arbitrarily chosen \( x \cdot y \) plane. We will see in Sec. V that this is actually the standard choice, and is covariant in the sense that we can transform any choice of \( x \cdot y \) plane into any other and hence also transform the codomain in a consistent fashion. As usual, when using a more geometric interpretation like this, the unit imaginary \( i \) that is found in standard treatments of spherical harmonics and angular momentum, and was used freely in Sec. II, will be replaced by a geometric object—in this case, the bivector representing the \( x \cdot y \) plane.

The codomain Straumann\(^{15} \) chose appears to be unique in the literature: for integer-weight SWSHs, he chose the codomain to be a two-dimensional subspace \( M \) of the Lie algebra \( \mathfrak{so}(3) \) = \( M \oplus \mathfrak{so}(2) \), where \( \mathfrak{so}(2) \) is the algebra corresponding to the fiber space \( S^1 \). In general the geometry behind this choice is not specified. However, when Straumann specializes to Euler angle coordinates, the \( \mathfrak{so}(2) \) fiber corresponds to an initial rotation about \( z \), so that \( M \) constitutes generators of rotations about \( x \) and \( y \). So in this presentation SWSHs take values in the space of vectors in the \( x \cdot y \) plane. This use of vectors instead of spinors is important to Straumann's approach, because it allows him to use familiar constructions in differential geometry. Of course, it is well known that spinor and vector representations of the plane are equivalent for quantities of integer spin,\(^{30} \) the underlying geometry of the codomain is the same in either case.

V. A NATURAL BASIS FOR SWSFS

We have determined that SWSFs are appropriately defined as functions from \( \text{Spin}(3) \) to the spinor algebra of two dimensions—familiar as the complex numbers \( \mathbb{C} \). The latter of these has various reasonable geometric interpretations, but the standard one involves the \( x \cdot y \) plane. In fact, Wigner\(^{17} \) introduced a canonical set of functions from \( \text{Spin}(3) \) to \( \mathbb{C} \), which are known as Wigner's \( \mathcal{D} \) matrices. Using the elements of these matrices, the standard SWSHs may now be redefined as
\[
y^{\ell, m}(R) := (-1)^s \sqrt{\frac{2\ell + 1}{4\pi}} \mathcal{D}_{m,-m}^{(\ell)}(R),
\] (21)

which is a slight extension of a formula already known to Goldberg \textit{et al.},\(^2 \) but here defining the SWSHs on \( \text{Spin}(3) \), rather than on coordinate systems of \( S^2 \). (Also note that the factor \((-1)^s\) differs from that of Goldberg \textit{et al.}, but is consistent with more modern standards.\(^{35} \)) Moreover, Bargmann\(^{35} \) and Gelfand, Minlos, and Shapiro\(^{36} \) proved that this collection of functions—encompassing all possible \( \ell, m, \) and \( s \) values—forms a complete orthogonal system in the space of square-integrable complex-valued functions on \( S^3 \). In this section we will first use Eq. (21) to briefly examine one benefit of defining SWSHs in this way, on the full spin group. We will see that these SWSHs transform among themselves, which cannot be said for the more standard SWSHs defined on coordinates of \( S^2 \). We will then derive the \( \mathcal{D} \) matrices using the geometric structure established by \( \text{Spin}(3) \), being careful about special cases, and suggesting improved methods for evaluating the necessary sums with greater numerical efficiency and accuracy. Finally, we will review the geometric features of SWSHs defined in this way, connecting back to the motivation mentioned in Sec. I relating to waves measured on a sphere.

A. Transforming SWSHs

Wigner constructed his \( \mathcal{D}^{(\ell)} \) matrices to form a representation of the spin group. That is, given \( R_1 \) and \( R_2 \) in \( \text{Spin}(3) \), we have
\[
\mathcal{D}^{(\ell)}_{m',m}(R_1 R_2) = \sum_{m''} \mathcal{D}^{(\ell)}_{m'',m'}(R_1) \mathcal{D}^{(\ell)}_{m',m''}(R_2).
\] (22)
This simple formula now allows us to relate SWSHs defined with respect to different frames. For example, if one frame is taken into the other by some rotation $R_1$ so that we can write $R_1 = R_d R_2$, we have

$$sY_{l,m}(R_1) = \sum_{m'} \mathcal{D}^{(f)}_{m,m'}(R_d) sY_{l,m'}(R_2).$$

(23)

The important feature of this equation is that the $\mathcal{D}^{(f)}_{m,m'}$ factors are all constant. That is, given $R_d$, these are complex coefficients independent of $R_1$ and $R_2$. So we can truly express $sY_{l,m}(R_1)$ as a finite and closed-form expansion in $sY_{l,m'}(R_2)$ for various values of $m'$. This is useful because it allows us to transform the value of a function given with respect to one frame into a different frame, which is a necessary step in some types of transformations, as explained in detail in Ref. 14.

It is important to note that there is no comparable transformation law when the $sY_{l,m}$ functions are defined on stereographic coordinates. In any case, the $(\theta_1, \varphi_1)$ rotations are restricted to special forms. Solving for $\gamma$, we get

$$\gamma = -2 \Im \log e^{\gamma}/e^{\gamma} \gamma = -2 i \log \left[e^{\gamma}/e^{\gamma} \gamma \right].$$

(25)

Of course, $(\theta_1, \varphi_1)$ and $(\theta_2, \varphi_2)$ are already related in a very complicated way when $R$ is anything other than a pure rotation about $z$. An equivalent result holds, of course, when SWSHs are defined on stereographic coordinates. In any case, $\gamma$ is a very complicated function of the coordinates—not just of the rotation. Because of this $\gamma$ function, it cannot be said that the $sY_{l,m}$ functions, when defined on coordinates of $S^2$, transform among themselves.

To be fair, we should note that while the SWSHs do not transform among themselves in this form, the modes of a spin-weighted function decomposed into SWSHs do transform among themselves under rotation. That is, if we have

$$s\gamma(\theta_1, \varphi_1) = \sum_{l,m} f_{l,m}(\theta_1, \varphi_1)$$

(26)

for some constants $f_{l,m}$, then we can use Eqs. (24) and (4) to see that the equivalent constants $f_{l,m}'$ defined with respect to a different basis are related by

$$f_{l,m}' = \sum_{m'} f_{l,m} \mathcal{D}^{(f)}_{m,m'}(R_d).$$

(27)

Note that this relationship depends only on the rotation $R_d$, and not on any coordinates. Naturally, the fact that the modes transform among themselves is extremely useful when treating only rotations. Unfortunately, it is not true when the transformation is more complicated—as with general Lorentz transformations.14

B. Defining Wigner’s $\mathcal{D}$ functions

As explained in Sec. IV, our SWSH functions will map into the spinor subalgebra of the $x$-$y$ plane. This subalgebra consists of linear combinations of the quaternion 1 and the quaternion representing the $x$-$y$ plane—which is actually $z^{-1}$. Our first task will be to decompose the SWSH function’s argument $R \in \text{Spin}(3)$ into two parts, each of which will be an element of this spinor subalgebra. We do this by taking parts of $R$ that are symmetric (do not change) and antisymmetric (change sign) under rotation by $\pi$ about the $z$ axis.

We can express the geometric notion of this rotation by the algebraic notion of conjugation by $z$—that is, multiplying on the left by $z$ and on the right by $z^{-1}$.38 The symmetric part of $R$ will be a linear combination of 1 and $z$, while the antisymmetric part will be a linear combination of $x$ and $y$. The latter can then be mapped into the same space as the former by multiplying on the left by $y^{-1}$, giving us two objects in the same two-dimensional spinor subalgebra—complex numbers, but with a geometric interpretation. Explicitly, we define

$$R_s := \frac{1}{2} \left( R + zRz^{-1} \right),$$

(28a)

$$R_a := \frac{1}{2} y^{-1} \left( R - zRz^{-1} \right).$$

(28b)
In terms of components, if $\mathbf{R} = R_1 \mathbf{1} + R_x \mathbf{x} + R_y \mathbf{y} + R_z \mathbf{z}$, we have

$$
R_x = R_1 + R_z \mathbf{z},
$$

(29a)

$$
R_z = R_y + R_x \mathbf{z}.
$$

(29b)

Noting that the coefficients are real numbers, while $z^2 = -1$, these quantities act precisely like complex numbers. This decomposition obeys an important product law: for any other quaternion $\mathbf{S}$, we have

$$
(\mathbf{RS})_x = R_x S_x - \bar{R}_a S_a,
$$

(30a)

$$
(\mathbf{RS})_z = R_x S_z + \bar{R}_a S_a.
$$

(30b)

We could, of course, accomplish a similar decomposition using any two orthogonal unit “pure-imaginary” quaternions in place of $\mathbf{z}$ and $\mathbf{y}$. The particular choices of Eq. (28) are made to correspond more directly with conventional presentations elsewhere. However, this choice must satisfy one important constraint: that the right-hand sides of Eq. (30) are linear combinations of $S_a$ and $\bar{S}_a$, rather than their complex conjugates. Furthermore, these equations should reduce to identities when either $\mathbf{R}$ or $\mathbf{S}$ is 1.

The derivation proceeds from here by constructing a $(2\ell + 1)$-dimensional vector space consisting of these spinors, where $\ell$ can be any non-negative integer or half-integer. Following Wigner, we can do this by providing a basis explicitly:

$$
e_{(m)}(\mathbf{S}) := \frac{S^{\ell+m} S^{\ell-m}}{\sqrt{(\ell+m)! (\ell-m)!}}.
$$

(31)

As usual, $m$ varies from $-\ell$ to $\ell$ in integer steps. We can also replace $\mathbf{S}$ with $\mathbf{RS}$ in this expression. The result can be expanded in terms of the original basis given here. We then define the $\mathfrak{D}$ matrix as the relevant expansion coefficients:

$$
e_{(m')}^{(\ell)}(\mathbf{R}) = \sum_m \mathfrak{D}_{m,m'}^{(\ell)}(\mathbf{R}) e_{(m)}(\mathbf{S}).
$$

(32)

We can expand the left-hand side here by inserting the right-hand sides of Eq. (30) into the right-hand side of Eq. (31). Since $\ell \pm m$ is always a non-negative integer, we can use the binomial theorem to expand each of the factors, then group the resulting terms to find the expansion coefficients $\mathfrak{D}_{m,m'}^{(\ell)}$ for this quantity. The naive calculation provides this expression, which (after accounting for minor differences in conventions) is the same as the formula given by Wigner. It is inefficient to calculate directly, and is subject to enormous errors or even arithmetic overflow—in which some of the factors are too large for computers to represent natively. We can refine the expression to be faster, more accurate, and deal with special cases efficiently.

We introduce four branches to the calculation of $\mathfrak{D}$, depending on the value of $\mathbf{R}$. First, we deal with the cases where either $|R_1| < \epsilon$ or $|R_1| < \epsilon$ for some small number $\epsilon$ comparable to machine precision. In either such case, we can ignore the smaller quantity and the product law (30) becomes simple. Then, depending on which component is smaller, $e_{(m')}^{(\ell)}(\mathbf{RS})$ is simply proportional to either $e_{(m')}^{(\ell)}(\mathbf{S})$ or $e_{(-m')}^{(\ell)}(\mathbf{S})$. If neither $|R_1|$ nor $|R_1|$ is small, we must use Eq. (33), but we can extract the constant terms, and express it as a polynomial in some constant. Here again, we distinguish between two cases, where we use the smaller of $|R_1/R_1|^2$ or $|R_2/R_1|^2$ as the expansion variable in which to express the polynomial. The polynomial should be evaluated using a generalization of Horner form [see Appendix A for more details] for improved speed and accuracy. Finally, the complex powers of the terms we factor out in these cases must be evaluated in a polar decomposition to avoid arithmetic overflow and to increase the speed of evaluation. For this purpose, we define the auxiliary variables

$$
r_\phi := |R_1|,
$$

(34a)

$$
r_\phi := |R_1|,
$$

(34b)

Functions are available in many standard software libraries to obtain both the modulus and argument simultaneously for increased accuracy and speed, and to translate back from this polar decomposition to the usual rectangular form of complex numbers.

Putting this all together, the result is that in practice it is best to calculate the $\mathfrak{D}$ matrices according to
Again, this expression is valid for integer or half-integer \( \ell \), and the sums are evaluated more quickly and accurately using the algorithm presented in Appendix A. [Note that \( \bar{z} \) has been replaced with \( i \) here, so as to not confuse the reader who has consulted this paper only for this equation. In any case, because they are algebraically identical, this form is likely to be more similar to the form in which the equation should be implemented in computer code.] The limits of the sums are

\[
\begin{align*}
\rho_1 &= \max(0, m' - m), \\
\rho_2 &= \min(\ell + m', \ell - m), \\
\rho_3 &= \max(0, -m' - m), \\
\rho_4 &= \min(\ell - m', \ell - m).
\end{align*}
\]

Unfortunately, because the sum alternates in sign, this is still numerically unstable for certain values of \( \mathbf{R} \) and \((\ell, m', m)\)—specifically, for \( r_s \approx r_a \) and \( m' \approx m \approx 0 \) when \( \ell \geq 12 \), as discussed further in Appendix A. If accurate values are needed for such values, these expressions can be used to initialize recursion relations,\(^{39}\) which are naturally independent of the parametrization of \( \mathcal{T} \) and can accurately determine the values of these elements with \( m' \approx m \approx 0 \).

C. Geometric interpretation of SWSHs and SWSFs

Now, equipped with a more detailed understanding of SWSFs, and a particular realization in the form of SWSHs, we can return to the issue of representing waves on a sphere \( S^2 \). We began with an arbitrary reference frame \((x, y, z)\). Using any element \( \mathbf{R} \) in the spin group \( \text{Spin}(3) \), we defined another frame

\[
\begin{align*}
\mathbf{a} &:= \mathbf{R} x \mathbf{R}^{-1}, \\
\mathbf{b} &:= \mathbf{R} y \mathbf{R}^{-1}, \\
\mathbf{n} &:= \mathbf{R} z \mathbf{R}^{-1}.
\end{align*}
\]

The space of all possible directions \( \mathbf{n} \) maps out the sphere, and the tangent plane at any such point is spanned by \( \mathbf{a} \) and \( \mathbf{b} \). Now, the first point to note is that a transverse wave must be given by some vector in the space spanned by \( \mathbf{a} \) and \( \mathbf{b} \), or some tensor or spinor constructed with those vectors. But we’ve expressed the SWSHs above as functions mapping into the spinor space of the \( x-y \) plane—that is, linear combinations of \( \mathbf{1} \) and \( \mathbf{z} \). So we may wonder how we can uniquely relate quantities in one space to quantities in another. Fortunately, \( \mathbf{R} \) gives us a solution to this problem: we simply rotate the \( x-y \) spinor via conjugation by \( \mathbf{R} \), just like with a vector.

An example will be helpful. Gravitational waves are typically modeled by a perturbation \( h^{\mu\nu} \) to the metric tensor, where the background metric is assumed to be Minkowski. Furthermore, the gauge can be chosen so that \( h^{\mu\nu} \) is traceless, and the perturbation is transverse to the direction in which the wave is traveling.\(^{40}\) This is then conventionally combined into a single complex number as\(^{41}\)

\[
\begin{align*}
h &:= \frac{1}{2} h^{\mu\nu} \left( (a_\mu a_\nu - b_\mu b_\nu) - i (a_\mu b_\nu + b_\mu a_\nu) \right), \\
&= h^{\mu\nu} \bar{m}_\mu \bar{m}_\nu.
\end{align*}
\]

In the second line we have used the vector \( \mathbf{m} \) defined in Eq. (3). The appearance of \( i \) explicitly in Eq. (38a) and implicitly in Eq. (38b) is conventional but not necessary; as always, the unit imaginary is generally best replaced by something with geometric significance.\(^{42}\) We used a geometric construction in Sec. V B to avoid the arbitrary introduction of the complex quantity \( i \), in favor
of \( z \). In particular, the value of a SWSH will be an element of the spinor space spanned by 1 and \( z \). But \( z \) has no direct geometric significance for an arbitrary point on the sphere or its tangent space. The more natural construction here is to replace \( i \) with \( n \). Now, if the value of the SWSH is \( \alpha + \beta z \) for some real numbers \( \alpha \) and \( \beta \), then we can write

\[
R(\alpha + \beta z)R^{-1} = \alpha + \beta n,
\]

which is a spinor of the \( a \cdot b \) plane, as desired. Conversely, we can use the inverse rotation to transform such a spinor back to the \( x \cdot y \) plane.

This well defined method of rotating the spinors explains another feature of our approach. To construct the SWSHs, we made a completely arbitrary choice of basis—in particular of the \( z \) vector that appears throughout Sec. V B. But the observed field we obtain at the end of this process (e.g., the gravitational-wave field \( h \)) is invariant under different choices of that basis. In particular, if we have a second basis \((x', y', z')\), there exists some rotation \( R_{i} \) such that

\[
x' = R_{i} x R_{i}^{-1}, \\
y' = R_{i} y R_{i}^{-1}, \\
z' = R_{i} z R_{i}^{-1}.
\]

We can then define \( R' := R R_{i}^{-1} \), so that

\[
a \equiv R' x' R'^{-1}, \\
b \equiv R' y' R'^{-1}, \\
n \equiv R' z' R'^{-1},
\]

where \( a, b, \) and \( n \) are precisely the same geometric objects found in Eq. (37). We can go through the entire process, simply replacing the unprimed basis vectors with their primed equivalent, evaluating the SWSHs and rotating by \( R' \) to get an element of the \( a \cdot b \) spinor space, and obtain precisely the same value. The result is invariant with respect to the choice of basis. Most importantly, we now have simple and well defined methods for computing and rotating SWSHs.

VI. THE DIFFERENTIAL OPERATOR \( \partial \) AND ANGULAR-MOMENTUM OPERATORS

In Sec. V B, we went to some lengths to express Wigner’s \( \Xi \) matrices directly in terms of quaternions, instead of their more traditional presentation in terms of Euler angles. The reason for this is that quaternions form the best presentation of both the rotation and spin groups: they are simpler and more intuitive to manipulate; they are more closely linked to the geometry they describe; they are free from singularities; and they are more efficient to compute with than angles. However, some of the more common tasks when analyzing spherical harmonics and related functions involve the angular-momentum operator. This is conventionally given in terms of Euler angles. It would be deeply unfortunate if we had to convert our function back to the Euler-angle presentation whenever we need to apply angular momentum operators. Instead, we will see that a simple geometric argument gives rise to the appropriate operators in terms of quaternions. We will also see another natural set of operators, and find that one of these is identical to the important spin-raising operator \( \partial \) defined by Newman and Penrose in their original description of spin-weighted spherical harmonics.

The familiar idea behind the angular-momentum operator is to find the rate of change in the value of a function defined on a sphere as one rotates around that sphere. More generally, for a function of a rotation operator, \( f(R) \), we wish to find the rate of change in the function as we apply infinitesimal rotations to \( R \). We first construct some rotation \( e^{i \epsilon j / 2} \) where \( \epsilon j \) is one of the standard unit basis vectors. We will apply this rotation to \( R \) and differentiate the function with respect to \( \theta \). That is, we define

\[
L_{j} f(R) := -i \frac{\partial}{\partial \theta} f \left( e^{i \epsilon j / 2} R \right) \bigg|_{\theta=0}.
\]

This coincides with our intuitive notion of the angular momentum operator evaluating the change in an infinitesimal rotation about a particular axis. We will show below that this is precisely the angular-momentum operator as found in the theory of the symmetric top.\(^{243}\) This is a slight generalization of the more familiar angular-momentum operator, which is usually seen as a differential operator acting on functions defined on the sphere \( S^{2} \); while this more general operator is defined for functions on \( S^{3} \), it also reduces to the simpler one. The particular form given here is even more unusual, however, in that it is not defined in terms of Euler angles, but directly in terms of elements of the spin group.

From a purely algebraic perspective the choice to apply the perturbing rotation by multiplying on the left seems fairly arbitrary. Arguments from geometric algebra\(^{30}\) suggest that the geometric interpretation for this algebraic operation of multiplication on the left is to model a physical rotation of the system; multiplication on the right corresponds to rotation of the basis with respect to
which the function is defined. For most physical applications, we are more interested in the former, which is why \( L_j \) as defined above is familiar to physicists. Of course, we have seen that spin-weighted functions depend explicitly on the basis, as shown in Eq. (4). So a variant form of the angular-momentum operator will also be useful for our purposes. We now define a comparable operator involving multiplication on the right:

\[
K_j f(R) := -z \frac{\partial}{\partial \theta} f \left( R e^{i\theta/2} \right) \bigg|_{\theta=0}.
\]

(43)

Note that the only difference between \( L_j \) and \( K_j \) is the order of multiplication inside the function argument. This operator measures the dependence of the function on the frame in which it was defined, which is not typically a useful notion in physics, so \( K_j \) is very uncommon in physics. Nonetheless, it is useful in the analysis of spin-weighted functions; we will see that it is (up to an overall sign) precisely the operator introduced by Goldberg et al.\(^2\)

To demonstrate equality between the \( L_j \) operator given here and the more common operator given in terms of Euler angles—or between \( K_j \) and the one given in terms of Euler angles by Goldberg et al.—we could express the quaternion argument \( R \) as a function of Euler angles, and compare the action of the operators and show that they must be equal for an arbitrary function. However, Euler angles are to be eschewed in all cases. A more relevant approach uses the fact that, as mentioned above, the function of Euler angles, and compare the action of the operators and show that they must be equal for an arbitrary function. As usual, we define the raising and lowering operators as \( L_\pm = L_x \pm z L_y \) and \( K_\pm = K_x \pm z K_y \). Straightforward evaluation with Eq. (33) shows that

\[
L_\pm \mathfrak{D}^{(f)}_{m',m}(R) = m' \mathfrak{D}^{(f)}_{m',m}(R),
\]

(44a)

\[
L_\pm \mathfrak{D}^{(f)}_{m',m}(R) = \sqrt{(\ell \pm m')(\ell \pm m') + 1} \mathfrak{D}^{(f)}_{m\pm 1,m}(R),
\]

(44b)

and similarly

\[
K_\pm \mathfrak{D}^{(f)}_{m',m}(R) = m \mathfrak{D}^{(f)}_{m',m}(R),
\]

(45a)

\[
K_\pm \mathfrak{D}^{(f)}_{m',m}(R) = \sqrt{(\ell \mp m)(\ell \pm m + 1)} \mathfrak{D}^{(f)}_{m',m \pm 1}(R).
\]

(45b)

These are—up to minor sign differences—the same expressions found elsewhere in the literature,\(^2,43\) showing that our geometric definitions of \( L_j \) and \( K_j \) are equivalent to previous definitions.\(^44\) With the definitions given here, there is no extraneous conversion to Euler coordinates on the spin group, for example.

Now, recalling that Eq. (21) defined the SWSHs in terms of \( \mathfrak{D}^{(f)}_{m',m}(R) \), and that the spin \( s \) of a SWSH corresponds to \(-m\), we see that \( K_+ \) is an index-raising operator, but a spin-lowering operator. Similarly, \( K_- \) is an index-lowering operator, but a spin-raising operator. These are important quantities in the literature on SWSHs, having been introduced by Newman and Penrose\(^1\) as \( \delta \) and \( \bar{\delta} \), respectively. We now extend to SWSHs defined on the spin group:

\[
\delta \left[ s Y_{\ell,m}(R) \right] = -K_- \left[ s Y_{\ell,m}(R) \right],
\]

(46a)

\[
\bar{\delta} \left[ s Y_{\ell,m}(R) \right] = K_+ \left[ s Y_{\ell,m}(R) \right].
\]

(46b)

These equations are true if we simply copy the original relations for \( \delta \) and \( \bar{\delta} \) acting on SWSHs from Newman and Penrose. However, because the factor of \((-1)^s\) in Eq. (21) differs from their convention, it might also be reasonable to incorporate an additional sign change.

Finally, we can define spin-weighted spherical functions generally. Acting on an arbitrary SWSH, we see that

\[
K_z s Y_{\ell,m}(R) = -s s Y_{\ell,m}(R).
\]

(47)

That is, \( s Y_{\ell,m} \) is an eigenfunction of \( K_z \), with eigenvalue \(-s\). Penrose and Rindler\(^6\) used a comparable relation involving the commutator \([\delta, \bar{\delta}]\) to define SWSHs, so we follow their example. We define a spin-weighted spherical function of weight \( s \) to be a function \( f \) taking arguments from the three-dimensional spin group and mapping to an associated two-dimensional Euclidean spinor space (which is isomorphic to \( \mathbb{C} \)) satisfying

\[
K_z s f = -s s f.
\]

(48)

The choice of a particular two-dimensional subspace selects a unique direction \( z \) orthogonal to it, which is enough to define the operator \( K_z \), making this definition independent of any particular frame chosen to express the functions concretely.
VII. CONCLUSIONS

This paper has shown that spin-weighted spherical functions (SWSFs) *cannot* be defined as functions on the sphere $S^2$. Section II established that the missing structure is a choice of fiducial direction in the tangent space to the sphere at each point. But topological restrictions complicate such choices, as shown in Sec. III. It turns out that the Hopf bundle provides the perfect structure for resolving these complications, simultaneously treating both the sphere $S^2$ and the alignment of its tangent spaces. The Hopf bundle is defined on the sphere $S^3$ (that is its “entire” space). This is also the topology of the spin group $\text{Spin}(3)$, but the group has additional structure allowing us to multiply elements and apply other manipulations. In particular, the quaternions were used to discuss the Hopf bundle more easily than the usual Cartesian presentation.

There is some subtlety regarding the use of the spin group rather than the rotation group $\text{SO}(3)$, but it is clear that either will suffice for the important cases of integer spin, while the spin group is needed for half-integer spin. Thus, the group of unit quaternions was proposed as the appropriate domain on which to define SWSFs. Furthermore, the codomain into which SWSFs should map was shown to be equivalently regarded as the complex numbers $\mathbb{C}$ or as the spinor space of the $x$-$y$ plane. The latter is more useful, because we can use a geometric construction to create the standard basis for SWSFs, known as spin-weighted spherical harmonics (SWSHs). These are closely related to Wigner’s $\mathbb{C}$ matrices, which we derived purely in terms of quaternions in Sec. V B. Then, we saw that the result can be uniquely rotated into the spinor space tangent to the sphere at a given point, and thus corresponds to a field propagating orthogonally to the sphere.

Having shown that SWSFs and SWSHs can be defined and described entirely within the intuitive and powerful framework of quaternions, Sec. VI then showed that angular momentum operators can be defined readily within the same framework. In particular, the standard $L$ operator is given by applying a rotation to the argument of a SWSF, and differentiating with respect to the size of that rotation. But this rotation is applied on the left; if the rotation is applied on the right, a distinct operator is found. It turns out that this operator $K$ is identical (up to minor quirks of conventions) to an operator introduced by Goldberg et al.\textsuperscript{2} As they showed, the ladder operators associated with $K$ are essentially the same as the spin-raising and -lowering operators $\delta$ and $\delta$ defined by Newman and Penrose in their original introduction of SWSHs.\textsuperscript{1}

Defining SWSFs as functions on the spin group first serves the basic function of actually providing a mathematically well posed formulation of SWSFs—an objective that has been surprisingly rare in the literature. But on a more practical level, it allows us to transform SWSFs. By using quaternions, we further provide a unified system that combines algebraic power, computational benefits, and geometric interpretations. For example, quaternions are a special case of the spacetime algebra\textsuperscript{46} which allows us to treat boosts and rotations in the same language. This approach was previously used to transform SWSHs under boosts\textsuperscript{45} by projecting the spacetime algebra down to quaternion components, and evaluating the SWSHs as functions of those quaternions. This is one example of the power and simplifications that result from defining SWSFs as functions of quaternions.

A related construction is that of tensorial spin-weighted spherical harmonics, which arise in various calculations for general relativity.\textsuperscript{46} Essentially, these harmonics are produced by coupling SWSFs to symmetric trace-free tensor fields; in particular, a basis is given by coupling the SWSFs to various tensor products involving the vector fields $\mathbf{n}$, $\mathbf{m}$, and $\mathbf{\bar{m}}$ defined above. As we’ve seen there are natural maps taking the spin group into these vector fields. Alternatively, simple tensor products can be constructed of multiple copies of $\mathbf{m}$, and the spin-weight of each such product lowered to give rise to the full variety of tensorial spin-weighted harmonics. But this requires applying $\delta$ to the tensor product, which in turn requires it to be defined on vector fields. Our definitions of $\delta$ relied on the angular-momentum operator $K_j$ given in Eq. (43), which is only defined on spinor fields. Fortunately, we can simply regard the vector fields as their equivalent quaternion fields, and the same formula applies, resulting in expressions identical to those found by Newman and Silva-Ortigoza.\textsuperscript{46} Thus, the tensorial SWSHs could also be coherently defined as functions from the spin group.

The final few paragraphs of Sec. VI (among others) illustrate that the various signs and other conventions lead into a confusing morass of inconsistent definitions when trying to compare results from different papers. In practice, the only reliable way to determine these conventions is to derive everything directly. The holistic approach of defining spin-weighted functions as functions on the spin group eases this difficulty by unifying the algebra with the geometry it represents.

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Appendix A: Evaluating polynomials with factorial and binomial coefficients

It is well known that polynomials should be evaluated numerically in Horner form, which is both faster and more accurate than naive direct evaluation. In this appendix, a few specializations of Horner form are presented, which can be used when the coefficients of the polynomial are factorials, or products and ratios of factorials—including binomials. These specializations work by calculating the coefficients themselves as part of the algorithm. In addition to the standard benefits of Horner-form evaluation, this speeds the computation of the coefficients and avoids arithmetic overflow when very large factorials are involved.

We first review the standard Horner form. Given a polynomial with coefficients $c_j$, the polynomial may be evaluated as

$$\sum_{j=j_1}^{j_2} c_j x^j = x^{j_1} \left[ c_{j_1} + x \left( c_{j_1+1} + x \left( c_{j_1+2} + \ldots \right) \right) \right].$$  \hspace{1cm} (A1)

Explicitly evaluating the left-hand side involves redundant calculations for the powers of $x$, since $x^j$ requires knowledge of $x^{j-1}$. The summation itself can also lead to delicate cancellations between terms, which can destroy numerical accuracy. If instead we evaluate the right-hand side, there is no redundant calculation of powers of $x$, and numerical accuracy is retained. This simple algorithm is given as follows.

1: $p = c_{j_1}$
2: $j = j_2 - 1$
3: while $j \geq j_1$ do
4: \hspace{1cm} $p = c_j + x \, p$
5: \hspace{1cm} $j = j - 1$
6: end while
7: $p = x^{j_1} \, p$

The final value of $p$ is the value of the polynomial. In this case, we need some way to obtain the values of the coefficients, which may be done by either indexing an array of precomputed coefficients or by using a function that computes the coefficient given the index.

Now, if the coefficient is a factorial in the summation index $j$, there is another redundancy, much like the redundancy in computing various powers of $x^j$. That is, computing $j!$ requires knowing $(j-1)!$, and so on. We can take advantage of this structure to find a more efficient expression. Generalizing slightly, we assume there is still some coefficient, but we have factored out a factorial:

$$\sum_{j=j_1}^{j_2} c_j j! x^j = j_1! x^{j_1} \left[ c_{j_1} + (j_1 + 1)x \left[ c_{j_1+1} + \ldots \right] \right].$$  \hspace{1cm} (A2)

Here, the algorithm is just slightly different; line 4 above becomes

4: \hspace{1cm} $p = c_j + (j + 1) x \, p$

and the final result in this case only will also need to be multiplied by $j_1!$.

It is a trivial task to modify this algorithm to compute the sum $\sum_j c_j (A + j)! x^j$. For our purposes, a more interesting sum is

$$\sum_{j=j_1}^{j_2} c_j \frac{(A + j)!}{(A + j)!} x^j = x^{j_1} \left( c_{j_1} + \frac{1}{A + j_1 + 1} x \left[ c_{j_1+1} + \ldots \right] \right),$$  \hspace{1cm} (A3)

for which line 4 in the algorithm becomes

4: \hspace{1cm} $p = c_j + \frac{1}{A + j + 1} x \, p$

An interesting modification occurs when the sign of $j$ is flipped in the factorial:

$$\sum_{j=j_1}^{j_2} c_j \frac{(B - j)!}{(B - j)!} x^j = x^{j_1} \left[ c_{j_1} + (B - j_1)x \left[ c_{j_1+1} + (B - j_1 - 1)x \left( c_{j_1+2} + \ldots \right) \right] \right],$$  \hspace{1cm} (A4)

in which case that line in the algorithm should be

4: \hspace{1cm} $p = c_j + (B - j) x \, p$

Note that we multiply by $B - j$, whereas we were dividing by $A + j + 1$ in the previous case.

The most important generalization of this algorithm applies to multiple factorials. For example, we can compute a polynomial with binomial coefficient as

$$\sum_j c_j \binom{C}{j} x^j = \binom{C}{j_1} \sum_j c_j \frac{j_1!(C - j_1)!}{j!(C - j)!} x^j,$$  \hspace{1cm} (A5)
using the same algorithm with
\[
4: \quad p = c_j + \frac{C^j}{j!^2} \times p
\]
and, of course, multiplying the final \( p \) by \( \left( \frac{c}{j!^2} \right) \).

For the purposes of this paper, it is interesting to apply this to computing elements of Wigner’s \( \Sigma \) matrices. The sum in question [depending on which branch is taken in Eq. (35)] looks something like this:

\[
\sum_{j=-\ell}^{\ell} \binom{\ell + m'}{\ell - m} \binom{\ell - m}{j} x^j = \binom{\ell + m'}{\ell - m} \sum_{j=\ell}^{\ell} \binom{\ell - m - j}{j} \binom{\ell - m - j}{j} \binom{\ell - m - j}{j} \binom{\ell - m - j}{j} ! \binom{\ell - m - j}{j} ! \binom{\ell - m - j}{j} ! \binom{\ell - m - j}{j} ! x^j. \tag{A6}
\]

Noting that the \( c_j \) coefficients in this case are all 1, this sum can be computed just as easily as the cases above using
\[
4: \quad p = 1 + \frac{\ell - m - j}{m' + m + j + 1} \frac{\ell - m - j}{j!} x \]

It is, of course, possible to use Horner’s rule to evaluate the polynomial directly, taking each coefficient as the appropriate binomial. However, that requires calculating two binomial coefficients at each step, which may be reasonably accomplished by indexing a pre-computed array of values. That, in turn, requires additional calculations to compute the index, as well as non-local operations in memory to retrieve the correct value.

Unfortunately, we can still find values for which the sum is not well conditioned, leading to a loss in accuracy when implemented either with Horner’s original algorithm or with this specialized algorithm. For example, if \( x \approx -1, \ell \) is large, and \( m' \approx -m \) is close to 0, then the coefficient \( \frac{\ell - m - j}{m' + m + j + 1} \frac{\ell - m - j}{j!} \) will vary dramatically as \( j \) changes. At some point during the loop over \( j \), this will bring the value of \( p \) very close to \(-1\), leading to rapid loss of accuracy in the sum. Perhaps even more importantly, there are simply many terms in the sum when \( \ell \) is large. This is never a problem for \( \ell \leq 12 \), because only one digit of precision is lost. For larger values of \( \ell \), however, we might expect these sums to lose up to \( \log_{10}(2^{\ell + 1}/\pi \ell) \) digits of accuracy—though that appears to overestimate the error by one or two digits when using this new algorithm. In any case, accuracy appears to be completely lost for certain values of \( x, m', m \) when \( \ell \) is as low as \( \ell \approx 60 \). If accurate values are needed for large \( \ell \), the results of this algorithm can be used as input to initialize recursion relations, which retain accuracy for all values of \( m \) and \( m' \).

**Appendix B: Parametrizing SWSFs**

In practice, when using SWSFs to describe radiation fields, we need a useful parametrization. We now discuss various parametrizations that can be used for this purpose, starting from a fairly general perspective. We want some parameter space \( P \) along with continuous maps \( e \) and \( b \) as given here:

\[
\begin{array}{c c c}
 & & \\
P & \downarrow e & b \\
S^3 & \rightarrow & \rightarrow S^2 \\
\end{array}
\tag{B1}
\]

Note that this diagram need not be commutative. Indeed, in some cases we will see that \( e \) may not be defined on all of \( P \). Ideally, we want \( e \) to be defined throughout \( P \) and injective (distinct elements in \( P \) map to distinct elements of \( S^3 \)), so that the spin-weighted function will be single-valued. We also want \( b \) to be surjective (for each element of \( S^2 \), there is some element of \( P \) that maps to it), so that the function can describe observations in each direction.

In Table 1, we collect a variety of common parametrizations along with their respective mappings. Perhaps surprisingly, the standard spherical coordinates provide one of the most useful parametrizations for SWSHs. They cover the entire sphere (\( b \) is surjective). And despite the well-known coordinate singularities at the north and south poles, each pair \((\theta, \varphi)\) corresponds to a unique element of the spin group (\( e \) is injective). These are the criteria mentioned above for a useful parametrization, which is why spherical coordinates may be chosen for implementations of numerical routines involving SWSHs—such as the state-of-the-art spinsfast package.

It is somewhat more common in the literature on SWSHs to find stereographic coordinates used. These have certain advantages over spherical coordinates, in that they are complex and so lend themselves to more elegant algebraic manipulations in many cases. However, inspection of the mappings shown in the table shows that \( b : P \rightarrow S^2 \) is only surjective when the point at infinity is included, but \( b : P \rightarrow S^3 \) is not defined at this point. In fact, it can be proven that such a mapping would again violate the Hairy-Ball Theorem. Thus, stereographic coordinates—at least in this simple form—do not provide a useful parametrization except for theoretical applications that do not require rigorous coverage of \( S^2 \).

Various related constructions may be more capable for certain purposes, such as using two complementary coordinate patches. The complications of implementing this construction are likely not worth the effort. The “homogeneous” stereographic coordinate
| Name | Parameter space $P$ | $e : P \rightarrow S^3$ | $b : P \rightarrow S^2$ |
|------|---------------------|--------------------------|--------------------------|
| Spherical coordinates of $S^2$ | $(\theta, \varphi) \in I \times S^1$ | $\exp \left[ \frac{y}{2} \right] \exp \left[ \frac{\varphi}{2} \right]$ | $(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ |
| Stereographic coordinates\(^{\text{a}}\) of $S^2$ | $\zeta \in \mathbb{C} \cup \{\infty\}$ | $\frac{1}{\sqrt{1 + \zeta \bar{\zeta}}} \left[ 1 + i \left( \frac{\zeta - \bar{\zeta}}{2} \right) x + \frac{\zeta + \bar{\zeta}}{2} y \right]$ | $\left( \frac{\zeta + \bar{\zeta}}{1 + \zeta \bar{\zeta}}, \frac{\zeta - \bar{\zeta}}{1 + \zeta \bar{\zeta}}, \frac{1 - \zeta^2}{1 + \zeta \bar{\zeta}} \right)$ |
| Homogeneous stereographic coordinates of $S^2$ | $(a + ib, c + id) \in \mathbb{C}^2 \setminus \{(0, 0)\}$ | $\frac{a + dx + cy + dz}{\sqrt{a^2 + b^2 + c^2 + d^2}}$ | $\frac{1}{r^2} \left( 2( ac + bd), 2(ad - bc), r^2 - 2(a^2 + b^2) \right)$ |
| Stereographic coordinates of $S^3$ | $(a, b, c) \in \mathbb{R}^3 \cup \{\infty\}$ | $\frac{1}{1 + r^2} \left[ 1 - r^2 + 2ax + 2by + 2cz \right]$ | $b \circ e$ |
| Quaternion logarithms | $(x, y, z) \in \mathbb{R}^3$ | $\exp[ax + yz] + [ay + xz]$ | $b \circ e$ |
| Euler angles | $(\alpha, \beta, \gamma) \in S^1 \times I \times S^1$ | $\exp \left[ \frac{\alpha}{2} \right] \exp \left[ \frac{\beta}{2} \right] \exp \left[ \frac{\gamma}{2} \right]$ | $b \circ e$ |
| Hyperspherical coordinates of $S^3$ | $(\psi, \theta, \phi) \in I \times S^1 \times S^1$ | $\exp \left[ \frac{\psi}{2} (x \sin \theta \cos \phi + y \sin \theta \sin \phi + z \cos \theta) \right]$ | $b \circ e$ |
| Hopf coordinates of $S^3$ | $(\eta, \zeta, \xi) \in I \times S^1 \times S^1$ | $\sin \eta(\cos \zeta + x \sin \zeta) + \cos \eta(y \cos \xi + z \sin \xi)$ | $b \circ e$ |
| Invertible quaternions | $(w, x, y, z) \in \mathbb{R}^4 \setminus \{0\}$ | $\frac{w + x \sin \zeta + y \cos \zeta + z \bar{\zeta}}{\sqrt{w^2 + x^2 + y^2 + z^2}}$ | $b \circ e$ |

\(^{\text{a}}\) These expressions are correct for projection from the south pole; it is more common to see projection from the north pole. This choice is made for consistency with our previous definitions, which give the points of the sphere as rotations of $z$ (the north pole).

\(^{\text{b}}\) This expression uses the quantity $r^2 := a^2 + b^2 + c^2 + d^2$ for compactness.

\(^{\text{c}}\) This expression uses the quantity $r^2 := a^2 + b^2 + c^2$ for compactness.

**TABLE I. Parametrizations of SWSFs.** We list a variety of parametrizations that can be used for SWSFs along with their mappings into $S^3$, considered to be parametrized by unit quaternions, and $S^2$ considered as a subset of $\mathbb{R}^3$. Note that for each of the parametrizations of $S^3$, we simply use the Hopf map of Eq. (14) to go from $S^3$ to $S^2$; this would also be possible for the parametrizations of $S^2$, but they are more normally defined directly.
system solves these problems using a pair of complex numbers, which are not both zero. Only their ratio is used, so this is the projective space \( \mathbb{CP}^1 \), which is topologically homeomorphic to \( S^2 \). This is the formulation favored by Eastwood and Tod. It is closely related to the 2-spinor formalism, which is in turn closely related to the quaternion formalism. In fact, the two complex components of the 2-spinor \((\pi_0, \pi_1)\) can be considered precisely the symmetric and antisymmetric parts of the quaternion \( \mathbb{R} \) under conjugation by \( z \) [see Eqs. (28)]. Then, the point on \( S^2 \) described by the stereographic coordinate \( \zeta = \pi_0/\pi_1 \) is precisely the same point as \( \mathbb{R} \times \mathbb{R}^{-1} \) (that is, the image of \( \mathbb{R} \) under the Hopf map). Numerous other parallels exist between quaternion algebra and the 2-spinor algebra, which may make it seem at first sight as though the homogeneous coordinates of \( \mathbb{CP}^1 \) are somehow equivalent to the quaternion representation. However, the projective operation loses information, and requires a choice of algebraic structure that is not inherently present in the quaternions.

A slight generalization of the usual stereographic coordinates of \( S^2 \) may be more relevant to our purposes, by representing \( S^3 \) directly. The stereographic projection generalizes to arbitrary dimensions, so the special case of \( S^3 \subset \mathbb{R}^4 \) is straightforward. Again, however, the point at infinity must be included in order for this to be a complete parametrization. In addition, the algebraic manipulations possible with complex numbers do not generalize very immediately to this system—though it is not entirely clear how much of a disadvantage that may be. On the other hand, the formulas involved in this parametrization are slightly simpler than those for the previous one.

In fact, the stereographic coordinates of \( S^3 \) may be shown to be a simple rescaling of the more familiar quaternion logarithms. These logarithms are the generators of rotation, and can be exponentiated to give unit quaternions. This exponentiation is periodic in the magnitude of the logarithm by \( 2\pi \), in precisely the same way as the usual complex logarithm is periodic by \( 2\pi \). Essentially, the logarithm is the compactified version of the stereographic coordinates of \( S^3 \), under the mapping

\[
(a, b, c) \mapsto (x, y, z) = (a, b, c) \frac{\arccos \frac{1-r^2}{r}}{r},
\]

where \( r = \sqrt{a^2 + b^2 + c^2} \). Clearly the quaternionic system is more computationally useful. Moreover, we recover algebraic niceties when using quaternions—potentially helpful for theoretical purposes. In fact, the quaternion logarithm is very closely identified with the axis-angle representation: the logarithm is just a unit vector along the axis, multiplied by one half the angle of the rotation.

We also have a set of three coordinate systems defined on \( P = S^1 \times I \times S^1 \) (or a permutation of those spaces): the Hopf, hyperspherical, and Euler coordinates. In each case, the coordinates are angles that are combined in different ways to arrive at a rotation. For example, the hyperspherical coordinates of \( S^3 \) are closely related to the axis-angle representation, where \( \psi \) represents the angle, and \((\theta, \phi)\) the spherical-coordinate direction of the axis. Unfortunately, all three systems share the same basic failing: they all provide non-injective mappings to \( S^3 \). In the case of the Euler angles, this well known problem is referred to as “gimbal lock.”

Finally, we come to what is clearly the preferred representation of rotations: quaternions. Quaternions contain clear geometric meaning that corresponds readily with the axis-angle understanding of rotations. They are free from coordinate singularity problems, and can simply be multiplied to express the composition of rotations. Their algebraic structure is as close as one may come to simple complex numbers, rather than real numbers. The result is essentially the same as the usual Riemann sphere \( \mathbb{C} \cup \{\infty\} \), except that the point at infinity is now treated in a more useful fashion. In particular, by representing the sphere in this way, the orthonormal frame is well defined at every point.

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10. The projective equivalence in this case is modulo nonzero complex numbers, rather than real numbers. The result is essentially the same as the usual Riemann sphere \( \mathbb{C} \cup \{\infty\} \), except that the point at infinity is now treated in a more useful fashion. In particular, by representing the sphere in this way, the orthonormal frame is well defined at every point.
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12. It turns out that the invertible quaternions can be reinterpreted as precisely \( \mathbb{C}^2 \setminus \{(0,0)\} \)—the space used by Eastwood and Tod before projection. In fact the two complex components are precisely the symmetric and antisymmetric parts of the quaternion defined in Eqs. (28). And the projective reduction of the complex components results in the same point on the sphere as the Hopf map of the equivalent quaternion, as given in Eq. (14). This correspondence is also described in more detail in Appendix B.
13. M. Boyle, L. E. Kidder, S. Ossokine, and H. P. Pfeiffer, “Gravitational-wave modes from precessing black-hole binaries,” (2014), arXiv:1409.4431 [gr-qc].
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Spin-weighted spherical functions

20

As is standard in geometry, the word “frame” is used here to refer to a basis along with an associated ordering of the basis elements. The same word is sometimes used in linear algebra to refer to a collection of vectors that need not be linearly independent. But the latter usage is not relevant for this paper, so it should not lead to any confusion.

Unfortunately, “orientation” is another word with two distinct meanings in closely related fields, but this word could cause some confusion. The sense we use here is the one used in mathematics, for which the orientation of a vector space is the choice of equivalence classes for the ordering of a basis (related to orientability of a surface). Another sense familiar to physicists may also be referred to as “angular position.” To avoid confusion, we reserve “orientation” for the first meaning and use “attitude” for the second meaning.

This notation already extends the usual definition of spin-weighted functions. These functions are normally written in terms of spherical coordinates as \( f(\theta, \phi) \) or in terms of complex stereographic coordinates as \( f(z) \). In those cases \( m \) is implicitly defined by the coordinate system. The latter notation is misleading, at best. Explicitly including \( m \) as seen here is an improvement, but we will find a better form below.

A final generalization uses tensor products of spinors in place of the tensor products of vectors, which allows for half-integer \( \ell \) and \( s \) values. We will allow for this most general case below. Very little is lost and much clarity is gained by describing the problem in terms of vectors at first.

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It is useful to show explicitly that \( S^2 \times S^1 \) and \( S^3 \) are indeed topologically distinct spaces. To see why, we can look at the fundamental groups of the spheres. We have \( \pi_1(S^1) \cong \mathbb{Z} \), and for \( n \neq 1 \) we have \( \pi_1(S^n) \cong \{0\} \). Since the fundamental group is a topological invariant, this shows that the two spaces cannot be homeomorphic. As a historical note, it is significant that this conclusion also follows from considering \( S^2 \); but not any higher homotopy groups. In particular \( \pi_2(S^3) \cong \mathbb{Z} \)—the proof of which was the surprising result from Hopf’s original introduction of this fiber bundle.

In Hopf’s original presentation,23 the order of the coordinates was slightly different; his form can be obtained from this one by swapping the \( x \) and \( y \) coordinates of \( S^1 \). The present ordering is adopted so that the quaternion mapping shown later will be more suited to other standard conventions.

C. Doran and A. Lasenby, Geometric algebra for physicists, 4th ed. (Cambridge Univ. Press, 2010).

This construction is essentially the same as the “flagpole” description of spinors,6 where \( b \) provides the pole and \( a \) provides the flag.

Again, it is useful to see that this truly is a distinct fiber bundle over the sphere. In this case, we merely need to show that \( S^3 \) and \( \mathbb{R}^3 \) are topologically distinct. But this is already known from the familiar fact that \( S^3 \cong SU(2) \) is simply connected, whereas \( SO(3) \) is not.16,24 In fact, with this construction, we have demonstrated that the Hopf bundle provides a “spin structure” over the bundle \( SO(3) \).22

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It turns out that the “vector” part of a quaternion would more accurately be described as a “bivector” part; we have simply followed tradition and used the same notation for vectors and bivectors. This is possible only by sheer coincidence and the fact that we work in three dimensions. This coincidence and the consequent confusion led to the quaternion-vector wars of the late nineteenth century,20 which may be the greatest mathematical tragedy in the history of physics. For our purposes, the important point is that the \( x-y \) plane is represented by the bivector \( x \wedge y \), which is traditionally denoted \( z \).

A full understanding of the geometry behind these operations requires Geometric Algebra (GA)10,23,24 which is, mathematically speaking, just Clifford Algebra (CA) over the field \( \mathbb{R} \). GA allows us to replace essentially all uses of complex numbers, quaternions, and more in physics (including quantum mechanics) with geometric constructions involving only real numbers.24 Moreover, through numerous publications over decades of work, Hestenes23,24 has provided GA with additional geometric interpretation that moves us beyond the mere formalism of CA. Through GA is a surprisingly elementary subject, explaining its relevance here would take us slightly beyond the scope of this paper, and yield little more of direct relevance than the basic complex and quaternion formalisms—those are just the first two nontrivial examples of GA.

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Clearly, under rotation of the tangent frame, \( h \) transforms with spin weight \( s = -1 \). Conversely, given \( h \), we can reconstruct the perturbation as \( h^\mu = h^m m^\mu \), which has no spin weight because it is a tensor. The complex “scalar” quantity \( h \) is able to contain all of this information because the gauge is chosen so that \( h^\mu \) is transverse, traceless, and symmetric.

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Note that Goldberg et al.2 defined \( K_l \) with a relative negative sign, and defined the corresponding spin raising and lowering operators with another relative sign and conjugation. That is, to reproduce their results, we would need to perform the translations \( K_l \leftrightarrow -K_l \) and \( K_s \leftrightarrow K_s \). Their choices appear to have been motivated by the curious negative sign in \( Y_{\ell m} \propto \mathcal{T}_{m,-} \). The choices here are made to enforce the symmetry between Eqs. (42) and (43), which leads to symmetry between Eqs. (44) and (45).

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