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The Spherical Harmonic Spectrum of a Function with Algebraic Singularities

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Abstract The asymptotic behaviour of the spectral coefficients of a function provides a useful diagnostic of its smoothness. On a spherical surface, we consider the coefficients a_l^m of fully normalised spherical harmonics of a function that is smooth except either at a point or on a line of colatitude, at which it has an algebraic singularity taking the form θ^p or $|\theta - \theta_0|^p$ respectively, where θ is the co-latitude and $p > -1$. It is proven that each type of singularity has a signature on the rotationally invariant energy spectrum, $E(l) = \sqrt{\sum_m (a_l^m)^2}$ where l and m are the spherical harmonic degree and order, of $l^{-(p+3/2)}$ or $l^{-(p+1)}$ respectively. This result is extended to any collection of finitely many point or (possibly intersecting) line singularities of arbitrary orientation: in such a case, it is shown that the overall behaviour of $E(l)$ is controlled by the gravest singularity. Several numerical examples are presented to illustrate the results. We discuss the generalisation of singularities on lines of colatitude to those on any closed curve on a spherical surface.

Keywords Spherical harmonics · Singularity · Spectrum · Algebraic decay · Darboux's principle

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1 Introduction

Spectral methods, or generalised Fourier series, approximate an unknown function by an expansion in terms of a prescribed set of basis functions which are usually

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orthogonal. The tail of the coefficient spectrum, showing how quickly the coefficients asymptotically decrease with increasing index, gives an important indication of how well any finitely truncated approximation is converged. Furthermore, this asymptotic scaling is often intimately linked with the location of singularities of the function: empirically determined spectra can therefore provide useful diagnostics about how and where the solution loses its differentiability, which may otherwise be difficult to obtain [7].

1.1 Functions in One Dimension

In one dimension, the Fourier basis set is the appropriate choice to represent periodic functions, whereas for non-periodic functions on the canonical interval $[-1, 1]$, Jacobi polynomials are optimal, of which particular examples are the well known Chebyshev or Legendre polynomials. In all these cases, for functions smooth except for singularities[1] away from the expansion interval in the complex plane, the coefficients are known to exhibit a geometric scaling of the form $\exp(-\mu n)$. Here, the integer n is the coefficient index and $\mu > 0$ is the location of the closest singularity, measured either by its imaginary coordinate in the Fourier case or the radial elliptical coordinate in the Jacobi case ([5], [23] pp. 245). If there are no singularities anywhere except at infinity (for instance, in the case of the exponential function), the coefficients decay super-geometrically.

Non-periodic functions on $[-1, 1]$ (on which we shall now focus) that have singularities located within the interval have an associated value of $\mu = 0$, and have spectral coefficients that decay only algebraically with n. In such cases the asymptotic scaling is limited not by the location (within this interval) of the singularities, but instead only by the structure of the most severe, a notion known as known as Darboux's principle [5]. The idea is simple: define a smooth function $g(x)$ by removing all singularities of f:

$$g(x) = f(x) - \sum_i f_i(x),$$

where $f_i(x)$ gives the dependence of the ith singularity. Since the spectra of f depends linearly on each of its constituent parts, and since g is smooth and therefore has an exponentially decaying spectrum, it follows that the spectra of f is dominated by the strongest singularity, which has associated the slowest algebraic spectral decay. This simple argument works well if there is a single gravest singularity; if there are multiple such, other methods may be required.

Such an algebraic scaling is straightforward to identify in a Chebyshev expansion of a function f which has only p well behaved derivatives at some $x_0 \in [-1, 1]$. Up to a normalisation factor, the coefficients are

$$a_n = \int_{-1}^{1} \frac{f(z)\,T_n(z)}{\sqrt{1-z^2}} dz = \int_0^{\pi} f(\cos\theta)\,\cos n\theta\, d\theta = \frac{1}{2}\int_0^{2\pi} f(\cos\theta)\,\cos n\theta\, d\theta \quad (1)$$

[1] I.e. branch points, fractional powers or poles, although examples of far more exotic singularities may be found in e.g. [6, 24].

using the relationship $T_n(\cos\theta) = \cos n\theta$. The rightmost quantity is simply the Fourier cosine transform of the symmetric function $f(\cos\theta)$. Integrating by parts p times we find

$$|a_n| = \frac{1}{2n^p} \int_0^{2\pi} f^{(p)}(\cos\theta) \left\{ \begin{matrix} \cos \\ \sin \end{matrix} \right\} n\theta \, d\theta, \tag{2}$$

the boundary terms vanishing by periodicity. Since the integral is bounded (by applying Cauchy's inequality), $|a_n| \le C\, n^{-p}$ where C is a constant.

Such arguments are very effective at placing algebraic upper bounds on the spectral coefficients, repeatedly integrating by parts until one of two things happen. Either a discontinuity in some derivative means that a boundary term does not vanish and so limits the asymptotic decay rate of a_n (this term rendering inconsequential any smaller contribution from any remaining integral), or the $(p+1)$st derivative ceases to be integrable and the terms after p integrations define an upper bound. The extension of this technique from Chebyshev polynomials to the much wider class of Jacobi polynomials is possible, either directly [20] or using their underlying differential equation [9]. However, such bounds are not necessarily tight; for example, $x^{1/3}$ cannot be integrated by parts more than once, but nevertheless has coefficients that decay as $n^{-4/3}$ by other arguments [5]. Functions that are analytic within $[-1, 1]$ have infinitely many derivatives and allow the above argument to be repeated infinitely many times: their coefficients a_n therefore decay to zero faster than any power of n, that is, they have exponential decay.

All members of the Jacobi polynomial family are known to exhibit exponential convergence for functions smooth on $[-1, 1]$ [23]. However, for functions that possess singularities on this interval there is no known such theory, general to all Jacobi polynomials, that provides an algebraic scaling of their coefficients. One complicating factor is that in certain special cases (in particular, as discussed shortly, singularities at the end points), Legendre and Chebyshev polynomials have coefficients that scale differently, despite singularities at interior points providing an identical scaling. There are several attempts in the literature to relate theoretically[2] Legendre and Chebyshev coefficients, for instance, by making assumptions on the derivatives of the function [3, 11]. An alternative and more pragmatic approach is simply to compare theoretical convergence results for specific basis sets, derived by comparison to the Fourier case [17, 18], contour integration [10, 16] or by applying asymptotic theory [22]. Expansions for common types of singularity, for a variety of basis sets, are summarised below [7]. However, before proceeding, we give the following definition:

Definition 1 A function has coefficients a_n that are said to scale as n^{-p}, denoted $a_n \sim n^{-p}$, if p is the largest real number for which

$$\limsup_{n\to\infty} \left| a_n\, n^p \right| < \infty.$$

[2] At least to within a factor of $\sqrt{n}$, although this can be removed by fully normalising the Legendre polynomials.

This statement defines the *envelope curve* for the coefficients as Cn^{-p}, for some constant C. For example, the two functional forms of $b_n = 10n^{-p}$ and $c_n = n^{-p}(1+\sin n)$ both scale in the same fashion as defined above.

Simple algebraic singularities at interior points $x_0 \in (-1,1)$ of the form $|x-x_0|^p$, for $p > -1$,[3] give rise to the scaling $a_n \sim n^{-(p+1)}$ for both (fully-normalised) Legendre and Chebyshev expansions. An identical result holds in the periodic case for a Fourier series, which can be extended to include a singularity of any of the forms

$$|x-x_0|^p, \qquad \operatorname{sgn}(x-x_0)\,|x-x_0|^p, \qquad H(x-x_0)\,|x-x_0|^p, \tag{3}$$

which all give rise to same scaling $a_n \sim n^{-(p+1)}$, where $\operatorname{sgn}(x) = x/|x|$ and the Heaviside function $H(x) = (\operatorname{sgn}(x)+1)/2$. These results may be further generalised by the multiplication of logarithmic terms: functions of the form $|x-x_0|^p \log|x-x_0|^q$ have coefficients that scale as $a_n \sim n^{-(p+1)} \log^q n$ [7, 18]. In this paper we shall consider the general class of singularities of order $p > -1$ of the form

$$\big(A + B\operatorname{sgn}(x-x_0)\big)\,|x-x_0|^p. \tag{4}$$

It can readily be verified that if f has a singularity of this form then

$$\frac{df}{dx} \sim p\operatorname{sgn}(x-x_0)\,\big(A+B\operatorname{sgn}(x-x_0)\big)\,|x-x_0|^{p-1} + 2B\delta(x-x_0)|x-x_0|^p$$

since $d|x|/dx = \operatorname{sgn}(x)$ and $d\operatorname{sgn}(x)/dx = 2\delta(x)$. If we further demand that $p > 0$, then df/dx has a singularity of order $p-1 > -1$ of the form (4) and an associated spectrum $a_n \sim n^{-p}$; the second term on the right is zero everywhere. Thus (4) is the appropriate generalised form of such singularities, with p giving the severity of the singularity and (A, B) prescribing the sign change and relative amplitude on either side of x_0.

A subset of singularities of this type are discontinuous integer derivatives. For example, if the third derivative of a function f has a finite jump at $x = x_0 \in (-1,1)$, that is, $f'''(x) \sim A + B\operatorname{sgn}(x-x_0)$ then f itself has a third order singularity of the form $(C + D\operatorname{sgn}(x-x_0))|x-x_0|^3$. In this paper, we only consider real functions and, since p may be non-integer, a dependence of $|x-x_0|^p$ rather than simply $(x-x_0)^p$ is mandatory. We remark that, if p is an even integer and $B = 0$ (a rather special case) then the singularity vanishes and the function is becomes analytic at x_0; if the function is otherwise smooth then the spectrum will decrease at a rate that is exponential rather than algebraic.

For the class of interior singularities of the form (4), both Legendre and Chebyshev polynomials have coefficients that scale identically. However, differences in the scaling emerge when considering singularities of order p at the end points of the domain $x = \pm 1$. Specific end point behaviour is unique to polynomial expansions: in the periodic case there is no such thing as an end-point: the integral is invariant

[3] The restriction $p > -1$ arises in order that the singularity is integrable, and so the integral of the function against any smooth basis function exists.

to translations of the interval over which the transform is taken. Singularities of the form $|x \pm 1|^p$ as $x \to \mp 1$ have associated (fully-normalised) Legendre coefficients that scale as $n^{-(2p+3/2)}$ [16] but Chebyshev coefficients that scale as $n^{-(2p+1)}$ [7]. Note also that the coefficients decay to zero twice as fast as a singularity of the same order at an interior point: the exponents being functions of $2p$ compared to p. In this sense, interior singularities are twice as severe as those at the end points.

1.2 Functions on a Spherical Surface

The focus of this paper is the extension of these one-dimensional results to a two-dimensional spherical surface. The basis functions we shall consider are the spherical harmonics, the natural choice in this geometry which have many optimal properties such as completeness and the uniform resolution of a function on a spherical surface [5]. Spherical harmonics,

$$Y_l^m(\theta,\phi) = P_l^m(\cos\theta)\begin{Bmatrix}\sin\\ \cos\end{Bmatrix} m\phi \tag{5}$$

where the integer indices l and m give respectively the degree and order, are each composed of a single Fourier mode in longitude and an associated Legendre function in colatitude $z = \cos\theta$. We shall adopt the full normalisation

$$\int_0^{2\pi}\int_0^{\pi}\left[Y_l^m(\theta,\phi)\right]^2 \sin\theta d\theta\, d\phi = 1 \tag{6}$$

in order to draw parallels with polynomials in one-dimension.

Spherical harmonics satisfy the second order eigenvalue equation

$$\nabla_1^2 Y_l^m = -l(l+1)Y_l^m \tag{7}$$

where ∇_1^2 is the surface Laplacian [2]

$$\nabla_1^2 = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}.$$

For a given function $f(\theta,\phi)$, we consider the properties of the expansion

$$f(\theta,\phi) = \sum_{m=0}^{\infty}\sum_{l=m}^{\infty} a_l^m\, Y_l^m(\theta,\phi)$$

where the sum over sine or cosine dependence in longitude is suppressed. Of primary interest will be to determine how a_l^m scales asymptotically as l and m both become large. The individual coefficients a_l^m depend on the orientation of the coordinate system and do not, themselves, have any particular physical meaning. However, the following lemma is fundamental to their utility:

Lemma 2 *The energy spectrum defined by*

$$E(l) = \sqrt{\sum_m \left[a_l^m\right]^2},$$

where the sum is taken over all harmonics of the same order, is invariant under arbitrary rotations of the coordinate system.

This follows from the invariance under rotations of the subspace of harmonics (homogeneous polynomials) of degree l, a result well known in quantum theory [e.g. 25]. In the context of geomagnetism, this spectrum (up to a pre-factor) is known as the Lowes-Mauersberger-Lucke spectrum [2]. We will ultimately be interested in the spectrum of functions possessing multiple singular structures which may have arbitrary orientation with respect to one another. Using this lemma, we may calculate the spectra associated with any single singularity in its natural coordinate system; the overall spectrum $E(l)$ can then be derived by appealing to the rotational invariance of each individual spectrum.

Just as their counterparts in one dimension discussed above, a function that is everywhere smooth on a spherical surface has an energy spectrum that converges at an exponential rate. This cannot be shown quite as tersely as before, since to integrate by parts (as in (2)), we would need an explicit (closed form) expression for the indefinite integral of Y_l^m with respect to both ϕ and $\cos\theta$. Unfortunately no such form is known (at least to the author's knowledge), although single integrals can be evaluated using recursion [15]. However, by exploiting the fact that spherical harmonics satisfy (7), we can iteratively integrate by parts twice by using Green's theorem [21] to show that

$$\left|a_l^m\right|^2 \le \left(l(l+1)\right)^{-2s} \oint \left|\left(\nabla_1^2\right)^s f\right|^2 d\Omega \tag{8}$$

where $d\Omega$ is the element of solid angle, so that $|a_l^m| \le C\, l^{-2s}$ for any integer s (since for smooth functions all the required derivatives exist), showing that the coefficients tend to zero faster than any algebraic power. If f has singularities in some derivative however, as before, this iterative process must terminate and we may show only algebraic convergence, $|a_l^m| \le C\, l^{-2q}$, for some integer $q > 0$. A limiting factor of this procedure is that only bounds of even-integer exponents arise for a_l^m. For example, for a singularity of the form $|\theta - \theta_0|^{5/2}$ we can use the integration-by-parts argument just once (since $(\nabla_1^2)^2 f$ is not square-integrable), so that $|a_l^m| \le C\, l^{-2}$; yet we will show below that $a_l^m \sim l^{-7/2}$ as $l \to \infty$ for fixed m, leading to $E(l) \sim l^{-7/2}$.

On $[-1, 1]$, a function can be singular only at a point, but in two-dimensions functions can also be singular on lines. In N-dimensional space, higher-order generalisations of points and lines render the landscape of possible singular structures even more complex. On a spherical surface, we consider singularities of two types: (i) point singularities and (ii) line singularities. In this paper, the latter type refers to singularities on lines of constant colatitude θ_0, in some rotated coordinate system, rather than a general closed curve. In the neighbourhood of such a line, a function which has a singularity of order p takes the form

$$\left(A + B\operatorname{sgn}(\theta - \theta_0)\right)|\theta - \theta_0|^p\, g(\phi)$$

for some real number $p > -1$ and smooth function $g(\phi)$. We will show that, by finding the asymptotic behaviour of the spectral coefficients a_l^m, the rotationally invariant spectrum scales as $E(l) \sim l^{-(p+1)}$. A point singularity at $\theta = 0$ (in some rotated system) takes the form θ^p and has an associated spectrum $E(l) \sim l^{-(p+3/2)}$. Intuitively, singularities on an entire curve should be more potent than a singularity of the same order but isolated at a point and should therefore lead to a slower decay of the energy spectrum; these results show that indeed this is the case.

By viewing line or point singularities within an appropriately oriented local 2D Cartesian coordinate system, we will show that there are strong links between the local Legendre (or Chebyshev or Fourier) spectrum and the global spherical harmonic energy spectrum. Singular lines of order p are locally equivalent to a singularity also of order p in only one variable (whose axis is locally perpendicular to the singular line) and, as such, its Legendre spectrum scales as $a_n \sim n^{-(p+1)}$, identical to the harmonic spectrum $E(l) \sim l^{-(p+1)}$. Close to a point singularity at $\theta = 0$, $|\theta|^p \approx |\sqrt{x^2 + y^2}|^p$ which is a 2D structure in the local Cartesian coordinates (which cannot be further reduced to a 1D singularity). Indeed, its 2D structure turns out to make it twice as singular as any particular 1D profile through the singularity: for example, on the line $x = 0$, the singularity takes the form $|y|^p$ whose Legendre spectra is $a_n \sim n^{-(2p+3/2)}$, whereas the global spectrum is $E(l) \sim l^{-(p+3/2)}$, equivalent to the signature of a 1D singularity of order $p/2$.

Just as in the one-dimensional case, we may consider a finite collection singular points and (of possibly intersecting) singular lines of arbitrary orientation; as we shall see, in the spirit of Darboux's principle, in most cases $E(l)$ depends only on the most grave. A complication arises when there are multiple gravest singularities since it is possible that the leading order behaviour of their sum exactly cancels out, leading to a spectrum that decays faster than expected. Although it is conjectured that such an occurrence is not possible, further investigation (and proof) is beyond the scope of this manuscript. However, a proof is supplied of a slightly weakened from of Darboux's principle which holds in all cases: $E(l)$ is bounded by the most grave singularity.

Lastly, we note that aspects of approximation theory somewhat parallel the development here. As discussed in Appendix B, the residual in the truncated expansion up to degree L

$$\sum_{l=L+1}^{\infty} E(l)^2 = R(L)^2 = \int \left| f(\theta, \phi) - \sum_{l=0}^{L} \sum_{m=0}^{l} a_l^m Y_l^m \right|^2 d\Omega \le C\, L^{-2(p+1/2)}, \quad (9)$$

if f has a line singularity of order p. If $p = 0$ then f is discontinuous and there will be an associated (possibly non-local) Gibbs effect, although this can be removed [4, 13]. This bound for $R(L)$ is entirely consistent with the scaling $E(l) \sim l^{-(p+1)}$. Since E converges at only an algebraic rate, $R(L)$ must decay slower than any particular $E(l)$ (see Appendix B). Note that, should $E(l)$ converge exponentially in l, then $R(L)$ would be well approximated by $E(L + 1)$ and we would anticipate that $R(L) \sim E(L)$.

The structure of the remainder of the paper is as follows. In the following section, we state and prove how algebraic singularities on points and lines translate into asymptotic scalings for $E(l)$. In Sect. 3 we provide several numerical examples that illustrate the key concepts, and end with a discussion in Sect. 4.

2 Main Results

The main results of this paper are stated below.

Theorem 3 *A function f is defined to have a line singularity of order p if, in some rotated coordinate system, within the neighbourhood of a line of colatitude $\theta = \theta_0 \in (0, \pi)$,*

$$f(\theta, \phi) \sim \big(A + B\operatorname{sgn}(\theta - \theta_0)\big)\, |\theta - \theta_0|^p\, g(\phi)$$

for some smooth $g(\phi)$, constants A and B and real $p > -1$. If we expand

$$f(\theta, \phi) = \sum a_l^m Y_l^m(\theta, \phi)$$

where the spherical harmonics have unit squared integral over all solid angle, then if f is smooth except on the singular line,

$$a_l^m \sim e^{-\alpha m}\, l^{-(p+1)} \quad \text{as } l, m \to \infty$$

with $\alpha > 0$ and $E(l) = \sqrt{\sum_m (a_l^m)^2} \sim l^{-(p+1)}$.

Theorem 4 *A function f has a point singularity of order $-1 < p \neq 0$ at $\theta = 0$ if*

$$f(\theta, \phi) \sim \theta^p.$$

If f is otherwise smooth, then

$$E(l) = a_l^0 \sim l^{-(p+3/2)} \quad \text{as } l \to \infty.$$

By invariance of $E(l)$ under rotations (Lemma 2), a point singularity anywhere on the spherical surface has such an energy spectrum.

Note that, as for any function f single valued at $\theta = 0$, $f(0, \phi)$ cannot depend on longitude so we may consider only the axisymmetric case. The special case $p = 0$ is specifically excluded above since there is no singularity.

It is also useful to remark that, despite appearances, even the innocuous looking function $f(\theta) = \theta = \cos^{-1} z$ is not smooth at $\theta = 0$. This can be identified in, for example, the fact that its gradient, $\nabla\theta = \mathbf{e}_\theta(\phi)$, is multivalued at $\theta = 0$.

Corollary 5 (Darboux's principle) *Suppose a function is smooth except for a finite number of point and line singularities of arbitrary orientation, the most grave of which has associated a spectral signature of l^{-p}. Then the overall behaviour of $E(l)$ is*

(i) *$E(l) \sim l^{-p}$ if there is a single gravest singularity (i.e. it is governed by the most grave) or*
(ii) *$E(l) \sim l^{-q}$ with $q > p$ if there are multiple gravest singularities (i.e. it is bounded by the most grave).*

The caveat in (ii) arises since it is possible that spectra associated with different singularities, each decaying as l^{-p}, could cancel at leading order, leaving a signature which decays faster than expected (although bounded by l^{-p}).

2.1 Outline of Proof for Line Singularities

Here we provide an outline of the proof of Theorem 1; much more detail can be found in Appendix A. Consider a function $f(\theta,\phi)$ that has a single line singularity of order p which, in an appropriately rotated coordinate system, takes the form

$$f(\theta,\phi) \sim \big(A + B\,\mathrm{sgn}(\theta-\theta_0)\big)\,|\theta-\theta_0|^p\, g(\phi)$$

in the neighbourhood of a line of colatitude $\theta = \theta_0 \in (0,\pi)$, for some smooth $g(\phi)$, constants A and B and real $p > -1$. We exploit the fact that the variables are separated in order to first transform in ϕ and then θ. In longitude, the structure is smooth and so a_l^m, for fixed l, converges exponentially fast in m. In latitude, we integrate by parts $2s$ times, where $-1 \le p - 2s \le 1$ (i.e. until integration by parts breaks down). This produces the bound $|a_l^m| \le C\,e^{-\alpha m}\,l^{-2s}$, where C is a constant and $0 < \alpha$, which is then tightened by exploiting the asymptotic structure of P_l^m for large l, to

$$a_l^m \sim e^{-\alpha m}\,l^{-(p+1)} \quad \text{as } l, m \to \infty.$$

The energy spectra

$$E(l) = \sqrt{\sum_m \big(a_l^m\big)^2} \sim l^{-(p+1)}$$

follows immediately.

This argument immediately extends to any finite number of singular lines which are all lines of colatitude with respect in the same coordinate system. The transform in longitude again must produce an exponentially decaying spectrum, and it only remains to transform in colatitude. By appealing to Darboux's principle in 1D, the overall spectrum is dominated by the gravest singularity. A further extension of this result to a finite number of arbitrarily oriented singular lines is given in Sect. 2.3.

2.2 Derivation of the Spectrum of Point Singularities

We consider a point singularity at $\theta = 0$, in the neighbourhood of which

$$f(\theta,\phi) \sim \theta^p$$

where $p > -1$. The axisymmetric spherical harmonic coefficients are given by an expansion in (fully normalised) Legendre polynomials

$$a_l^0 = \int_0^\pi \theta^p\, P_n(\cos\theta)\sin\theta\, d\theta = \int_{-1}^1 \big[\cos^{-1} z\big]^p\, P_n(z)\, dz, \tag{10}$$

on changing variable to $z = \cos\theta$. In order to derive the scaling, we make recourse to the known result (proven in [16]):

Lemma 6 *The (fully normalised) Legendre coefficients of a function possessing an end point singularity of the form* $|x \pm 1|^p$ *scale as*

$$a_n \sim n^{-(2p+3/2)}.$$

Although (10) is written in algebraic form, it is not immediately apparent what order the singularity takes in the variable z, since $\cos^{-1}$ is itself singular at the end points. As discussed in Appendix A, by smoothness of $\cos^{-1} z$ at interior points, if any function $h(\theta)$ has a singularity of order p at $\theta \in (0, \pi)$, then so does $h(\cos^{-1} z)$ at $\cos\theta_0 \in (-1, 1)$. That is, the change of variable simply effects a coordinate stretch and leaves invariant the order of the singularity. However, at the end points $z = \pm 1$, $\cos^{-1}$ has infinite slope and alters the nature of the singularity. Let us consider the behaviour of $\cos^{-1} z$ close to $z = 1$. Let $\epsilon = 1 - z$, $0 < \epsilon \ll 1$; since $\cos\epsilon \sim 1 - \epsilon^2/2$, then $\cos\epsilon^{1/2} \sim 1 - \epsilon/2$ and so

$$\left[\cos^{-1}(1-\epsilon)\right]^p \sim (2\epsilon)^{p/2}.$$

Thus within a neighbourhood of $z = 1$, the singularity in (10) is of order $p/2$ rather than p; applying Lemma 6 gives $a_l^0 = E(l) \sim l^{-(p+3/2)}$.

2.3 The Extension to a Finite Collection of Singularities

We now consider a function which has a finite number of (possibly intersecting) line and point singularities of arbitrary orientation. Key to the derivations above for a single singularity treated in isolation was that, after an appropriate rotation of the coordinate system, we were able to exploit separation of variables to integrate first in ϕ and then in θ. However, this breaks down when f has two or more singular structures (lines or points) which are arbitrarily orientated. Nevertheless, by exploiting knowledge of the spectra of each component part, we will show that a weak form of Darboux's principle still applies: the gravest singularity (point or line) bounds the energy spectra.

Consider the case of a function with two singularities: $f(\theta,\phi) = f_a(\theta,\phi) + f_b(\theta,\phi)$, where $f_a(\theta,\phi)$ and $f_b(\theta,\phi)$ are individually smooth except on either a line or point. Let the spherical harmonic coefficients of f_a and f_b be a_l^m and b_l^m respectively, and suppose their energy spectra scale as

$$E_a(l) \sim l^{-k_a}, \qquad E_b(l) \sim l^{-k_b}.$$

Let us first consider the case with $k_a < k_b$: that is, there is a single gravest singularity (associated with k_a in this case). By linearity, the spherical harmonic coefficients of f are $a_l^m + b_l^m$ and the energy spectrum is

$$E_{a+b}(l)^2 = \sum_{m=0}^{l} \left(a_l^m + b_l^m\right)^2 = \sum_{m=0}^{l} \left(a_l^m\right)^2 + \left(b_l^m\right)^2 + 2a_l^m b_l^m. \tag{11}$$

By Cauchy's inequality,

$$\sum_{m=0}^{l} a_l^m\, b_l^m \le \sqrt{\sum_{m=0}^{l} \left(a_l^m\right)^2 \sum_{m=0}^{l} \left(b_l^m\right)^2} \le C\, l^{-(k_a+k_b)}, \tag{12}$$

where C is a constant, a term bounded by a singularity intermediate between those of f_a and f_b (and so has no influence asymptotically relative to k_a). It follows from (11) that

$$E_{a+b}(l) \sim l^{-k_a} \tag{13}$$

is governed by the gravest of the two singularities.

The case of $k_a = k_b$ is more difficult, as the bound (12) then scales in the same fashion as the two other terms in (11). If this bound happens to be tight, it is conceivable that a rather special cancellation takes effect at leading order so that $E_{a+b}(l)$ decays faster than l^{-k_a}. If such a cancellation were to arise, the scaling of the total energy would not be given by (13) but governed by a higher-order term in the asymptotic series of the terms in (11). Any resulting scaling of $E_{a+b}(l)$ will, of course, be bounded above by l^{-k_a}, since each term in (11) is similarly bounded. It is clear that this weak version of Darboux's principle can be extended to a finite collection of arbitrarily orientated singular lines or arbitrarily located singular points.

Such a delicate cancellation would, if it occurred, be equivalent to the notion that, in the spectral signature, the sum of two singular functions would not be "as singular" as either of its constituents. It is conjectured below that such an occurrence is not possible. If this supposition is true, then the stronger form of Darboux's principle in Corollary 5(i) would hold in general, irrespective of the number of gravest singularities.

Conjecture 7 *Suppose that $f = \sum_i f_i$, where the sum is over a finite set of functions f_i, each possessing a single singularity on the spherical surface of either point or line type, having associated a spectral signature of l^{-p}. Then the energy spectrum of f decays as $E \sim l^{-p}$.*

A thorough investigation of this issue is beyond the scope of this manuscript, and indeed is almost certainly tied to a rigorous proof of Darboux's principle in 1D (which has only yet been proven for Taylor series and not for generalised expansions [5]).

Whether or not the special cancellation arises is really a question of the uniqueness of the leading order behaviour of the spectrum of a singularity. Note that for the simple case of the cancellation between two spectra (each associated with a distinct singularity), it is not sufficient that they possess the same asymptotic scaling: $a_l^m \sim b_l^m$, but moreover that the coefficients of the leading order behaviour must be identical. That is, if the complete description of the dominant spectral signatures of the singularities were determined to be $h_a(l)\, l^{-k_a}$, i.e. $|a_l^m(l) - h_a(l)\, l^{-k_a}| = o(l^{-k_a})$ for some function h_a at fixed m (and similarly for f_b), it would have to be the case that $h_a(l) + h_b(l) = 0$ for all $l > L$ for some L. The sum $a_l^m + b_l^m$ would then lose its l^{-k_a} leading-order behaviour and scale according to a faster-decaying term in its asymptotic series. It is argued below that such an occurrence is unlikely; but no proof is provided and the conjecture remains an open question.

Consider the case of two line or two point singularities of different orientation but of the same order. On the spherical surface, since the singularities are related by a rotation, it follows that $\mathbf{a} = M\mathbf{b}$ where $\mathbf{a}$ and $\mathbf{b}$ are vectors of the coefficients a_l^m and b_l^m, and M represents the rotation in spectral space (such a matrix always exists as, for fixed truncation, the set of spherical harmonics is closed under rotations). For a rotation of arbitrary angle, the matrix M mixes up the order and degree of the coefficients, and for any given l and m, as empirical tests show, in general b_l^m bears little resemblance to a_l^m, let alone has the same asymptotic scaling. Thus barring the trivial rotation (where M is the identity matrix) the required cancellation is seemingly unlikely. Singularities on two lines which are parallel reduces (after transforming in longitude) to the usual 1D application of Darboux's theorem in latitude, generally believed to be valid. Lastly, as demonstrated by example (Fig. 1) in the next section, the functions h_a and h_b related to the spectral signature of a point and line singularity respectively are very different: $h_a(l)$ is close to a constant, whereas $h_b(l)$ has considerably more structure. Thus it would seem unlikely that two singularities could ever be arranged to effect this special cancellation.

3 Examples

We now present some examples which illustrate the scaling laws derived above. The spherical harmonic coefficients of any given function can be computed numerically using an FFT in the longitudinal direction and Gaussian-quadrature in the latitudinal direction; having found the coefficients, it is straightforward to compute the energy spectrum $E(l)$. To ensure numerical accuracy, we increase the resolution of the transforms and the number of abscissae used until the coefficients converge.

As a first example, Fig. 1 shows the spectra of an axisymmetric point and line singularity of orders 1 and 3/2 respectively:

$$f_1(\theta) = 100\theta \cos\theta, \qquad f_2(\theta) = \cos\theta\, |\theta - 1|^{3/2}$$

both of which give $E(l) \sim l^{-5/2}$. In each case, the (converged) spectra have been computed up to degree 400 using 1000 Gaussian quadrature points. We have deliberately included a factor of 100 in f_1 for graphical purposes. Note that although the spectrum for f_1 fits almost exactly an algebraic form for all l plotted, for f_2, $E(l)$ only gives the scaling of the envelope. Because of chance cancellations, some coefficients are smaller than the scaling law suggests. It is worth remarking that, because of the vast difference in spectral structure, it is unlikely that any two similar such singularities have spectra that sum to zero (to leading order).

The identical scaling of the spectra of the given point and line singularity is illustrative of a more general fact: if only the asymptotic spectral scaling of a function is given as l^{-k}, it is not possible to discriminate between a causal point singularity of order $l^{k-3/2}$ or a line singularity of order l^{k-1}.

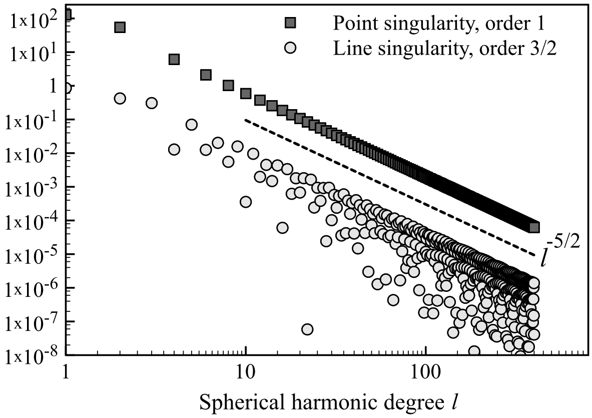

Fig. 1 A comparison of the spherical harmonic spectra $E(l)$ of a point singularity of order 1 and a line singularity of order 3/2 as defined in the text; in both cases $E(l) \sim l^{-5/2}$

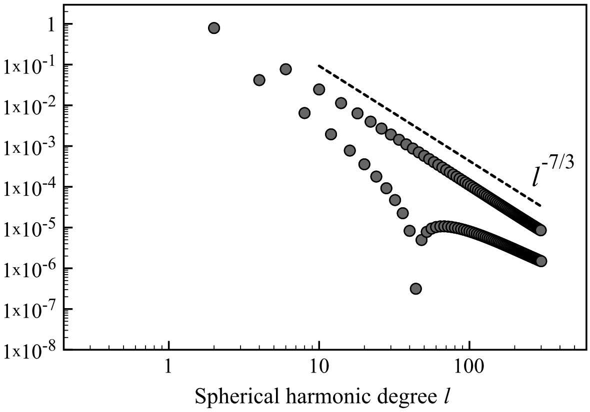

Fig. 2 The energy spectrum $E(l)$ of a function which has two line singularities of order $p = 4/3$: on the lines of intersection between the planes $z = 0$ and $y = 0$ with the unit spherical surface centred at the origin. The *dashed line* confirms that the envelope scales as $l^{-7/3}$

A second example illustrates intersecting line singularities. We consider the function

$$\left|\theta - \frac{\pi}{2}\right|^{4/3} + \left|\cos^{-1}(\sin\theta\,\cos\phi) - \frac{\pi}{2}\right|^{4/3} = \left|\cos^{-1} z - \frac{\pi}{2}\right|^{4/3} + \left|\cos^{-1} y - \frac{\pi}{2}\right|^{4/3}$$

where we have expressed the dependence in Cartesian coordinates on the right, assuming that the spherical surface is of unit radius. The first term has a singularity on the equatorial line $\cos\theta = z = 0$ of order $p = 4/3$, the line of intersection of the plane $z = 0$ and a spherical surface. The second term is simply the first term rotated by $\pi/2$ about the x-axis: the line of intersection of the plane $y = \sin\theta\cos\phi = 0$ and the spherical surface. Figure 2 confirms the envelope slope of $l^{-7/3}$, computed using maximum spherical harmonic degree and order of 400 and 1500 abscissae in both latitude and longitude.

Lastly, as addressed in the discussion, we speculate that the results pertaining to the spectral signature of a line singularity may be generalised to any closed curve on the spherical surface. To demonstrate that this a reasonable assertion, we present a

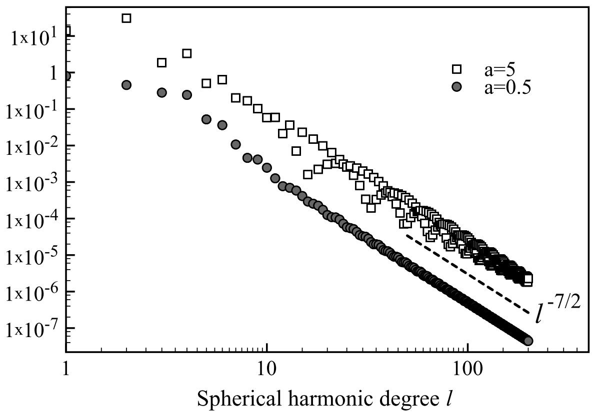

Fig. 3 The spectrum $E(l)$ of f_3 which has a nonlinear line singularity of order $p = 5/2$ on the intersection of the surface $1/2 + ay - z^3 = 0$ with the unit spherical surface centred at the origin, for $a = 1/2$ and $a = 5$. The *dashed line* confirms that, for both choices of a, the envelope scales as $l^{-7/2}$

third example of the function

$$f_3(\theta, \phi) = |1/2 + a \sin\theta \cos\phi - \cos^n \theta|^{5/2},$$

where $n \geq 0$ and for some real a. If $n = 1$, then the singularity occurs on the intersection of the plane $1/2 + ay - z = 0$ with the spherical surface, that is, on a line of colatitude in some coordinate system (if $a = 0$ then this is simply the line $\theta = \pi/3$). We consider the nonlinear case $n = 3$: the curve $1/2 + ay - z^3$ is the intersection of a cubic plane curve with the spherical surface and is therefore closed. Figure 3 shows that $E(l) \sim l^{-7/2}$ when $a = 1/2$ and $a = 5$; for these restricted cases we therefore verify the proposed extension to Theorem 1. It is worth remarking that when constructing such examples some care must be taken to avoid introducing unwanted non-regular behaviour at the poles (at which the coordinate system is singular); in this case it is achieved by ensuring all variables have an explicit Cartesian representation.

4 Discussion

In this paper we have discussed the spherical harmonic signature of either line or point (or both) singularities, of specified order, of an otherwise smooth function. Line singularities are more grave than point singularities of the same order, a fact that is entirely consistent with the fact that line and point singularities are topologically distinct. The results in this paper have been proved using a mixture of asymptotic analysis and recourse to standard results. A more formal treatment of this work is almost certainly possible, perhaps by extending the analysis of [22] to associated Legendre functions and spherical harmonics.

We speculate that the spectral signature of a singularity defined on a line of colatitude (in some coordinate system) may be extended to that of a singularity on *any* closed curve on the spherical surface, since such a curve can be smoothly mapped to a line of colatitude. In Sect. 3 we provided a numerical example that shows the validity of this assertion in the given case. Such a generalisation may be intuitive but a proof does not appear to be straightforward. On the interval $[-1, 1]$, if $f(x)$ has a singularity of order p at $g(x_0)$, then $f(g(x))$ has a singularity of order p at x_0, if g is a smooth (possibly nonlinear) bijective function on $[-1,1]$ (see Appendix A). Since $f(x)$ and $f(g(x))$ have singularities of the same order, it follows that they possess the same asymptotic scaling of (say) Legendre polynomial coefficients. This statement is equivalent to showing that

$$\int_{-1}^{1} P_n(x)f(x)dx \sim \int_{-1}^{1} P_n(x)f\big(g(x)\big)dx = \int_{-1}^{1} P_n\big(g^{-1}(y)\big)f(y)J(y)dy$$

where $y=g(x)$ and J is the associated Jacobian of transformation. To prove this assertion, the key problem is that, in the variable y, although f now appears untransformed, $P_n(g^{-1}(y))$ are no longer Legendre polynomials and we cannot say anything further about how the integral scales with n. The same issue occurs on a spherical surface: the smooth mapping that connects any closed curve with a line of colatitude corrupts the spherical harmonics, and the results that we have derived cannot be directly applied. However, in both one and two dimensions, crude estimates of the scalings may still be obtained using integration by parts.

One powerful application of spectral methods, as pointed out in the introduction, is the ability to use the rate of decay of the spectrum to probe any singular behaviour of the function. However, such a procedure is, in the most general case, plagued with non-uniqueness. Firstly, with knowledge of only the asymptotic scaling of the spectrum $E(l)\sim l^{-k}$, it is not possible to discriminate between the cause being a point singularity of order $l^{k-3/2}$ or a line singularity of order l^{k-1}. It is worth remarking that such a degeneracy is a generic issue; for example, in atmospheric turbulence it is not possible to say definitively which are the controlling singularities [12], there being two distinct scalings in the energy spectrum of n^{-3} and $n^{-5/3}$ on different ranges of the spatial wavenumber n. Secondly, only a weakened form of Darboux's principle could be proven here, so that the overall spectral slope supplies only a bound on any individual component singularities. This bound will not be tight if two or more singularities have spectra which sum together in such a way that a delicate cancellation takes place at leading order, leaving the total spectrum decaying faster than expected. However, this circumstance is conjectured never to arise, so that the overall spectral slope is precisely that stemming from any gravest singularity. Further work on this subject is beyond the present scope, and may be advanced by the derivation of a formal proof of Darboux's principle in 1D.

Lastly, it is worth highlighting a particular example in which much can be learned from the energy spectrum (which is, in fact, the motivating example for this manuscript). Low-viscosity flow in a rotating spherical shell leads to shear layers on the tangent cylinder, the axial cylinder of fluid that is tangent to the inner spherical boundary [19]. In the absence of viscosity, such shear layers become formal discontinuities. The spherical harmonic spectrum of such solutions will have a signature dictated by the order of the singularities on the tangent cylinder, which are lines of colatitude on any spherical surface. In this physical system it is likely that these are the only singularities present, so it is possible, assuming that Darboux's principle holds in the stronger form, to discern the order of the line singularities solely from the spectrum.

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Appendix A: The Spectral Signature of Line Singularities

Consider a function $f(\theta,\phi)$ that has a single line singularity of order p which, in an appropriately rotated coordinate system, takes the form

$$f(\theta,\phi) \sim \big(A + B\operatorname{sgn}(\theta-\theta_0)\big)\,|\theta-\theta_0|^p\, g(\phi) \tag{14}$$

in the neighbourhood of a line of colatitude $\theta=\theta_0\in(0,\pi)$, for some smooth $g(\phi)$, constants A and B and real $p>-1$. We will show that the asymptotic form of the spherical harmonic coefficients takes the form

$$a_l^m \sim e^{-\alpha m}\, l^{-(p+1)} \quad \text{as } l, m \to \infty,$$

with $0<\alpha$, from which the energy spectra

$$E(l) = \sqrt{\sum_m \big(a_l^m\big)^2} \sim l^{-(p+1)}$$

follows.

Before embarking on a proof, we first show that if $f(\theta,\phi)$ has a singularity of order p on $\theta=\theta_0$, and if $\theta=h(z)$ is a smooth invertible (possibly nonlinear) function with $\theta_0=h(z_0)$, then $f(h(z),\phi)$ has a singularity of order p on the line $z=z_0$. That is, this smooth coordinate transformation leaves invariant the order of the singularity. Close to $z=z_0$, $\theta=h(z)\sim h(z_0)+(z-z_0)h'(z_0)$ and so $\theta-\theta_0\sim(z-z_0)h'(z_0)$. It follows that, provided $h'(z_0)$ is finite,

$$f\big(h(z),\phi\big) \sim \big(C + D\operatorname{sgn}(z-z_0)\big)\,|z-z_0|^p\, g(\phi),$$

and so $f(h(z),\phi)$ has a singularity of order p as $z\to z_0$. If $h'(z_0)$ is not finite, then the singularity in the independent variable z may take a different form from that in θ (see Sect. 2.2).

To prove the result required, it is marginally easier to work with the transformed coordinate $z=\cos\theta$. The singularity in θ of order p, as defined above, translates into a singularity of the same order in z since the inverse cosine function, away from its end points, is smooth. The associated Legendre functions satisfy the Sturm-Liouville equation (where $z=\cos\theta$)

$$\mathcal{L}_m P_l^m(z) = l(l+1)\, P_l^m(z),$$

where

$$\mathcal{L}_m u = -\frac{d}{dz}\left(\big(1-z^2\big)\frac{du}{dz}\right) + \frac{m^2}{1-z^2}\, u(z).$$

For a given spherical harmonic order m, let us transform first in azimuth

$$f_m(\theta) = \int_0^{2\pi} f(\theta,\phi) \left\{ \begin{matrix} \sin \\ \cos \end{matrix} \right\} m\phi \, d\phi. \tag{15}$$

By assumption, g is smooth and so f_m decays exponentially fast in m as $e^{-\alpha m}$, $\alpha > 0$. It only remains to transform f_m in colatitude. Since our spherical harmonics are fully normalised,

$$a_l^m = \int_{-1}^{1} P_l^m(z)\, f_m(z) dz = \frac{1}{l(l+1)} \int_{-1}^{1} \mathcal{L}_m P_l^m(z)\, f_m(z) dz. \tag{16}$$

Let the (unique) integer s be such that

$$-1 < p' \le 1, \qquad p' = p - 2s.$$

Under the assumptions on f, we can integrate by parts twice, s times [9], to find that

$$a_l^m = \frac{1}{[l(l+1)]^s} \int_{-1}^{1} \mathcal{L}_m^s f_m(z)\, P_l^m(z) dz. \tag{17}$$

We now exploit the asymptotic behaviour of associated Legendre functions in the open interval $(-1, 1)$ [1]:

$$P_l^m(\cos\theta) \sim \left(\frac{\pi^2(\delta_{m0}+1)}{2} \sin\theta \right)^{-1/2} \cos\bigl((l+1/2)\theta - \pi/4 + m\pi/2\bigr) + O\bigl(l^{-1}\bigr) \tag{18}$$

which, in accordance with (6), are normalised such that

$$\int_{-1}^{1} \bigl[P_l^m(z) dz\bigr]^2 dz \sim \bigl(\pi(\delta_{m0}+1)\bigr)^{-1}. \tag{19}$$

Provided that $\mathcal{L}_m^s f_m$ is integrable (as we shall justify shortly), and noting from (18) that $P_l^m(\cos\theta)\sin\theta$ is bounded for $l \gg 1$, it follows that

$$|a_l^m| \le \frac{1}{[l(l+1)]^s} \int_0^{\pi} \bigl|\mathcal{L}_m^s f_m(\cos\theta)\bigr| \bigl|P_l^m(\cos\theta)\sin\theta\bigr| d\theta \le C\, l^{-2s}. \tag{20}$$

The function $\mathcal{L}_m^s f_m$ has an (integrable) singularity of order $-1 < p - 2s$ at $z = \cos\theta_0$. The only other place where it might fail to be integrable is at the end points, $z = \pm 1$, due to repeated multiplications by the factor $1/(1-z^2)$ in $\mathcal{L}_m^s$. However, f_m is not just any function: since f is smooth away from the singular line, f_m must behave as $\sin^m\theta$ as $\theta \to 0, \pi$ [5] and in fact the end points present no trouble. Indeed, writing $f_m(z) = (1-z^2)^{m/2} w(z)$ for some $w(z)$,

$$\begin{aligned} &\mathcal{L}_m\bigl[\bigl(1-z^2\bigr)^{m/2} w(z)\bigr] \\ &\quad = \bigl(1-z^2\bigr)^{m/2}\bigl[\bigl(z^2-1\bigr) w''(z) + 2(1+k) z\, w'(z) + m(m+1)\, w(z)\bigr], \end{aligned} \tag{21}$$

so that $\mathcal{L}_m f_m$ also has an mth order zero; iterating, we see that $L_m^s f_m(z)$ does as well and so remains regular at $z = \pm 1$.

To tighten the bound on a_l^m from l^{-2s} (20), we now use (18) again. In view of the quasi-trigonometric form of (18), one might be tempted to apply directly the Fourier convergence theory, summarised in the introduction, to (14). However, this is not possible, due primarily to the error term in (18), swamping any scaling that decays more rapidly than $O(l^{-1})$. We therefore only use (18) to tighten the scaling we already have.

We divide the remaining analysis into two cases depending on the sign of p'. Let us denote $\mathcal{L}_m^s f_m(z) = q_m(z)$, where $q_m(z)$ has a zero of order m at $z = \pm 1$ and a singularity of order $-1 < p' \leq 1$ at $\cos\theta_0$.

Case I: $-1 < p' \leq 0$

Direct substitution of (18) into (17) gives

$$\frac{(l(l+1))^s\, a_l^m}{C} \sim \int_0^\pi q_m(\cos\theta)\sqrt{\sin\theta}\cos\left((l+1/2)\theta - \frac{\pi}{4} + \frac{m\pi}{2}\right)d\theta + O\big(l^{-1}\big), \tag{22}$$

where $C = (\pi^2(\delta_{m0}+1)/2)^{-1/2}$. Formally, since the asymptotic expansion is valid only away from the end points, we should restrict attention to the interval $[-1+\epsilon, 1-\epsilon]$ for some $0 < \epsilon \ll 1$, modifying the limits of integration in (22). However, in view of the non-singular nature of the integrand in (22) near the end points, we may take ϵ to be so small so that the error incurred by altering the interval to $[-1, 1]$ can be neglected. The function $q_m(\cos\theta)\sqrt{\sin\theta}$ is smooth except for (i) a zero of order $m + 1/2$ at $\theta = 0$ and (ii) a singularity at θ_0 of order $p' \leq 0$. Since the singularity (ii) is more potent than (i), it therefore dominates the spectrum. Furthermore, noting that the above is just a (shifted) cosine transform, we may appeal to the Fourier results summarised in the introduction to see that, for some $\alpha > 0$,

$$a_l^m \sim e^{-\alpha m}\, l^{-2s}\,(l+1/2)^{-(p'+1)} \sim e^{-\alpha m}\, l^{-(p+1)}.$$

Case II: $0 < p' \leq 1$

We cannot use the same argument as above as not only might the zero of order $m + 1/2$ at $\theta = 0$ have a stronger influence than the singularity at θ_0, but $l^{-(p'+1)} < l^{-1}$ and the dominating error term means that we cannot do better than the bound l^{-2s-1}. Instead we integrate (17) by parts once (rather than twice) to find

$$\begin{aligned}\big(l(l+1)\big)^s\, a_l^m &= \frac{1}{l(l+1)}\int_{-1}^1 \big(1-z^2\big)\frac{dq_m(z)}{dz}\frac{dP_l^m(z)}{dz}dz \\ &\quad + \frac{m^2}{l(l+1)}\int_{-1}^1 \frac{q_m(z)\,P_l^m(z)}{1-z^2}\,dz\end{aligned}$$

the boundary term vanishing as both q_m and dP_l^m/dz are nonsingular at $z = \pm 1$ and everywhere continuous. Now we use the recurrence [1, 8.5.4]

$$\big(1-z^2\big)\frac{dP_l^m}{dz} = Q(l)\,(l+m)P_{l-1}^m - lzP_l^m \sim l\big(P_{l-1}^m - zP_l^m\big)$$

if $l \gg m$, which has been adjusted to take into account the normalisation (19) by inserting the algebraic factor $Q(l)$, where $Q(l) \to 1$ as $l \to \infty$. It follows that, when $l \gg m$:

$$\big(l(l+1)\big)^s a_l^m \sim \frac{1}{(l+1)} \int_{-1}^{1} \frac{dq_m(z)}{dz} \big(P_{l-1}^m - zP_l^m\big) dz + \frac{m^2}{l(l+1)} \int_{-1}^{1} \frac{q_m(z)\, P_l^m(z)}{1-z^2} dz.$$

Since dq_m/dz has a singularity of order $p'-1$ with $-1 < p'-1 \le 0$, it follows that by appealing to case I, the first integral (without the prefactor) scales as $l^{-((p'-1)+1)}$. The second integral (without the prefactor) scales algebraically in l with exponent either $-(p'+1)$ or -1 (from the error term in (18)), which ever is the greater. Since $p' > 0$ then the entire second term scales as l^{-3}. Note that despite the factor of $(1-z^2)$ in the denominator, this integral always exists: if $m = 0$ then it is trivially zero; if $m > 0$ then both P_l^m and q_m behave like $(1-z^2)^{m/2}$ as $z \to \pm 1$ and so the integrand is everywhere finite. Since the entire first term scales as $l^{-(p'+1)}$, it follows that $a_l^m \sim e^{-\alpha m}\, l^{-2s-p'-1} = e^{-\alpha m}\, l^{-(p+1)}$, $\alpha > 0$.

The entire analysis can be generalised to the case with singularities of the form $(A + B\operatorname{sgn}(\theta-\theta_0))|\theta-\theta_0|^p \log|\theta-\theta_0|^q$, by applying standard Fourier results [5, 18]. In such a case, $a_l^m \sim e^{-\alpha m}\, l^{-(p+1)} \log^q l$, $\alpha > 0$.

Lastly, we show that the energy spectra, binned per degree l, takes the form

$$E(l) = \sqrt{\sum_m \big(a_l^m\big)^2} \sim l^{-(p+1)}$$

as $l \to \infty$ when $a_l^m \sim e^{-\alpha m} f(l)$ for some dependence $f(l)$. Since the sum over m converges exponentially, its sum scales independently of l:

$$E(l)^2 \sim f^2(l) \sum_{m=0}^{l} e^{-2\alpha m} \sim f^2(l)\, \frac{1-e^{-2\alpha l}}{1-e^{-2\alpha}} \sim f^2(l),$$

and the result follows.

Appendix B: Application of Approximation Theory

We summarise here some relevant results from approximation theory that somewhat parallel the development given in the paper. For ease of explanation, we frame most of the discussion in terms of a Legendre polynomial representation in 1D. We consider on the interval $[-1, 1]$

$$R(N)^2 = \int_{-1}^{1} \big(u(x) - P_N u\big)^2 dx = \sum_{n=N+1}^{\infty} a_n^2, \tag{23}$$

a measure of the residual incurred in approximating u by its truncated expansion in (fully normalised) Legendre polynomials to degree N, $P_N = \sum_{n=0}^{N} a_n P_n(x)$. Let us define

$$\|f\|_{H^m}^2 = \sum_{r=0}^{m} \int_{-1}^{1} \left(\frac{d^r f}{dx^r}\right)^2 dx,$$

the Sobolev norm of f involving derivatives of up to degree m. It may be shown that

$$R(N) \le C N^{-m} \|u\|_{H^m} \tag{24}$$

for any m for which $\|u\|_{H^m}^2$ exists [8, 9], placing algebraic bounds on $R(N)$ depending on the differentiability of u. Using space interpolation, it is possible to extend this bound to non-integer values of m, which may also be generalised to approximations in other orthogonal polynomials.

Of relevance here is to consider a function u with a singularity of the form $|x - x_0|^p$, for some real $p > -1$. In the introduction of this paper, we summarised results that showed that $a_N \sim N^{-(p+1)}$. It is of interest to investigate what the comparable bound on $R(N)$ would be. It is straightforward to see that the $(p + 1/2)$ derivative of u (using the interpolation between integer derivatives) has a singularity of the form $|x - x_0|^{-1/2}$ which is not square-integrable, although u has a finite H^m norm for any $m < p + 1/2$. Taking the supremum of these values (assuming C is independent of m) leads to $R(N) \le C\, N^{-(p+1/2)}$.

This bound for $R(N)$ is entirely consistent with that for $a_N \sim N^{-(p+1)}$. Since a_N converges at only an algebraic rate, $a_N/a_{N+1} \to 1$ as $N \to \infty$ from which it follows that $a_N/a_{N+n} \to 1$ for any integer $n > 0$ and so all a_n, $n > N$, asymptotically "equally contribute" to the residual. Thus $R(N)$ must decay slower than any particular a_n. Note that, should a_n converge exponentially in n, then $R(N)$ would be well approximated by a_{N+1} and we would anticipate that $R(N) \sim a_N$.

These one-dimensional results have exact counterparts for functions defined on a spherical surface. It may be shown that

$$R(L) = \sqrt{\oint \left| f(\theta,\phi) - \sum_{l=0}^{L} \sum_{m=0}^{l} a_l^m Y_l^m \right|^2 d\Omega} \le C L^{-m} \|f\|_{H^m}$$

where H^m is defined in an analogous manner [14]. For functions which have singularities on lines of colatitude of the form $|\theta - \theta_0|^p$, we may therefore infer the bound $R(L) \le C\, L^{-(p+1/2)}$.

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