Appendices

A.1 Hyperspherical Harmonics

The following reproduces notes of Professor Mark Dennis on the derivation of hyperspherical harmonics in hyperspherical coordinates via Gegenbauer polynomials. It is this analytic form that we use in our numerical investigation of the 3-sphere, introduced in Sect. 1.7.2 and explained in Chap. 2, though other representations would be equivalent under an appropriate weighting.

We here describe some of the coordinate systems for the 3-sphere based on straightforward generalization of the 2-sphere, and the spherical harmonics, defined as the natural orthonormal eigenfunctions of the Laplace-Beltrami operator on the 3-sphere.

Most simply, the (unit) 3-sphere in 4-dimensional euclidean space with cartesian position (x, y, z, w) is defined as the locus

$$x^2 + y^2 + z^2 + w^2 = 1.$$

Positions on the 3-sphere are specified by three angles, ϕ, θ and ψ, with $0 \le \theta, \psi \le \pi$ and $0 \le \phi < 2\pi$, in a way generalizing the coordinates of the 2-sphere:

$$\begin{aligned} w &= \cos\psi, \\ z &= \sin\psi\cos\theta, \\ x &= \sin\psi\sin\theta\cos\phi, \\ y &= \sin\psi\sin\theta\sin\phi, \end{aligned}$$

which clearly satisfies the 3-sphere condition. Clearly, the 'equator' with $w = 0$, $\psi = \pi/2$ corresponds to a regular 2-sphere with coordinates θ, ϕ.

We also frequently use 'complex coordinates' u, v for the 3-sphere, with

$$u \equiv w + \mathrm{i}\,z, \qquad v \equiv x + \mathrm{i}\,y,$$

A.J. Taylor, *Analysis of Quantised Vortex Tangle*,
Springer Theses, DOI 10.1007/978-3-319-48556-0

clearly therefore satisfying $|u|^2 + |v|^2 = 1$. In particular, the argument of v is ϕ, which is useful in identifying $e^{i\ell\phi}$ behaviour in 3-sphere harmonics.

The most frequent representation of the 3-sphere (or the group of 3D rotations/SU(2), which has the 3-sphere or a related space as its group manifold) is by 'stereographic projection' into regular 3D euclidean space with position $\boldsymbol{R} = (X, Y, Z)$, most conveniently with the assignment $\boldsymbol{R} \equiv \tan\psi/2(\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta)$, i.e. like usual spherical coordinates with $R = \tan\psi/2$. This can be thought of as 'south-pole projection' of the w-axis of the 3-sphere, as may be readily checked from the complex coordinates assignment

$$u = \frac{1 - R^2 + 2\,\mathrm{i}\,Z}{1 + R^2}, \qquad v = \frac{2(X + \mathrm{i}\,Y)}{1 + R^2}.$$

We note it has often been convenient in previous work to use north-pole projection ($\mathrm{Re}\,u = (R^2 - 1)/(R^2 + 1)$), which would lead to $\cot\psi/2$ in the stereographic projection of our chosen angles; we adopt south-pole projection here.

These different coordinates give rise to a metric

$$\begin{aligned} ds^2 &= g_{ij}dx^i dx^j \\ &= d\psi^2 + \sin^2\psi(d\theta^2 + \sin^2\theta d\phi^2) \\ &= \frac{4}{(1+R^2)^2}\left(dR^2 + R^2(d\theta^2 + \sin^2\theta d\phi^2)\right), \end{aligned}$$

which has volume element $\sin^2\psi\sin\theta\,\mathrm{d}\psi\,\mathrm{d}\theta\,\mathrm{d}\phi$ (or, stereographically projected, $8(1+R^2)^{-3}R^2\sin^2\theta\,\mathrm{d}R\,\mathrm{d}\theta\,\mathrm{d}\phi$), yielding a volume of $2\pi^2$.

This metric allows the Laplace-Beltrami operator Δ to be defined (we use Δ rather than ∇^2 as we are on a curved manifold), where as usual $g = \det g_{ij}$,

$$\begin{aligned} \Delta &= \frac{1}{\sqrt{g}}\partial_i\left(\sqrt{g}g^{ij}\partial_j\right) \\ &= \frac{1}{\sin^2\psi}\partial_\psi(\sin^2\psi\partial_\psi) + \frac{1}{\sin^2\psi}\left(\frac{1}{\sin\theta}\partial_\theta(\sin\theta\partial_\theta) + \frac{1}{\sin^2\theta}\partial^2_\phi\right), \end{aligned}$$

where in the last line, the term in large brackets is the usual laplacian on the 2-sphere.

We now deduce the form of a natural set of eigenfunctions of Δ in $\psi\theta\phi$ coordinates. Since the regular 2-sphere laplacian occurs in our expression for Δ, we assume the desired functions have the form

$$\mathcal{Y}_{n,\ell,m}(\psi,\theta,\phi) = \Psi^\ell_n(\psi)\,\sin^\ell\psi\,Y^m_\ell(\theta,\phi),$$

for the usual spherical harmonics $Y^m_\ell(\theta,\phi)$, which are orthonormal on the 2-sphere and have eigenvalue $-\ell(\ell+1)$, with $2\ell+1$-fold degeneracy. The $\sin^\ell\psi$ factor has been included following the angular forms of x, y, z above: each Y^m_ℓ can be expressed as an order-ℓ complex homogeneous polynomial of cartesian coordinates on the 2-sphere.

Writing $c \equiv \cos\psi$, $\Psi(\psi) = X(c)$, we can rewrite

$$\begin{aligned}\Delta\mathcal{Y} &= \frac{Y_\ell^m}{1-c^2}\left(-\sqrt{1-c^2}\partial_c\{-(1-c^2)^{3/2}\partial_c\}[(1-c^2)^{\ell/2}X(c)] - \ell(\ell+1)(1-c^2)^{\ell/2}X(c)\right) \\ &= (1-c^2)^{\ell/2}Y_\ell^m\left[(1-c^2)X'' - (2\ell+3)cX' - \ell(\ell+2)X\right],\end{aligned}$$

and recognising the similarity of the last line with the Gegenbauer differential equation

$$(1-x^2)y'' - (2a+1)xy' + n(n+2a)y = 0$$

whose solutions are the Gegenbauer polynomials $C_n^{(a)}(x)$, we conclude that

$$\mathcal{Y}_{n,\ell,m}(\psi,\theta,\phi) = \sqrt{\frac{2^{2\ell+1}n!(1+\ell+n)}{\pi(1+2\ell+n)}}\ell!\sin^\ell\psi C_n^{\ell+1}(\cos\psi)Y_\ell^m(\theta,\phi),$$

where the appropriate Gegenbauer normalization factor has been included. We thus have

$$\Delta\mathcal{Y}_{n,\ell,m}(\psi,\theta,\phi) = -(n+\ell)(n+\ell+2)\mathcal{Y}_{n,\ell,m}(\psi,\theta,\phi),$$

so the eigenvalue is (unsurprisingly) labelled by $n+\ell \equiv N$, and we rewrite

$$\boxed{\mathcal{Y}_{N\ell m}(\psi,\theta,\phi) = \sqrt{\frac{2^{2\ell+1}(N-\ell)!(1+N)}{\pi(1+\ell+N)!}}\ell!\sin^\ell\psi C_{N-\ell}^{\ell+1}(\cos\psi)Y_\ell^m(\theta,\phi),}$$

with Laplace-Beltrami eigenvalue $N(N+2)$. Since each ℓ is $2\ell+1$-fold degenerate, the total degeneracy for the eigenvalue labelled by N is

$$\sum_{\ell=0}^{N}(2\ell+1) = (1+N)^2.$$

A.2 A Random Walk Construction

We give here the algorithmic details of generating closed random walks via the method of [1]. A full explanation of the mathematical details and relevant proofs is given in this original source.

The algorithm in the general case returns an unbiased random walk of N linear segments (which therefore generically fails to close by some random distance), from the space of all random walks with a beta-distribution on edge lengths which is mapped to the $(4N+1)$-sphere. The algorithm is as follows:

- Select at random a point on the $(4N+1)$-sphere, i.e. an array of $4N$ real entries with modulus 1.
- Partition the vector as N sets of 4 numbers. Each of these is identified as the real, i, j and k components of a quaternion; we label them p_1, p_2, p_3 and p_4.
- Convert each quaternion to a point on the 2-sphere via the Hopf map. In practical terms, the x, y and z Cartesian positions are given by

$$x = p_1^2 + p_2^2 - p_3^2 - p_4^2 \, , \tag{A.1}$$

$$y = 2(p_2 p_3 - p_1 p_4) \, , \tag{A.2}$$

$$z = 2(p_1 p_3 - p_2 p_4) \, . \tag{A.3}$$

- Each of these positions defines one edge of the random walk, of length $\sqrt{x^2 + y^2 + z^2}$. Recover the random curve by joining edges as sequential vectors.

To create a closed curve, as we need for an investigation of knotting and comparison with our vortices, [1] isolate positions on the $(4N-1)$-sphere corresponding to random walks that end with distance 0 from their origin. The above algorithm is modified to select only such points via a construction of complex numbers, as follows:

- Generate two orthogonal Gaussian random vectors with scalar product zero, each of N entries. By first generating two independent Gaussian random vectors labelled $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$, we orthogonalise these as

$$\boldsymbol{u}_f = \boldsymbol{u}_i / \sqrt{|\boldsymbol{u}_i|^2} \, , \tag{A.4}$$

$$\boldsymbol{v}_1 = \boldsymbol{v}_i - \boldsymbol{u}_f^* \cdot \boldsymbol{u}_f \, , \tag{A.5}$$

$$\boldsymbol{v}_f = \boldsymbol{v}_1 / \sqrt{|\boldsymbol{v}_1|^2} \, , \tag{A.6}$$

  such that $\boldsymbol{u}_f$ and $\boldsymbol{v}_f$ are normalised and orthogonal.
- Perform the Hopf map on these components to retrieve a set of edges. This now has the form

$$x = \mathrm{Re}(\boldsymbol{u}_f \cdot \boldsymbol{u}_f^* - \boldsymbol{v}_f \cdot \boldsymbol{v}_f^*) \, , \tag{A.7}$$

$$y = \mathrm{Re}(i(\boldsymbol{u}_f \cdot \boldsymbol{v}_f^* - \boldsymbol{v}_f \cdot \boldsymbol{u}_f^*)) \, , \tag{A.8}$$

$$z = \mathrm{Re}(\boldsymbol{u}_f \cdot \boldsymbol{v}_f^* + \boldsymbol{v}_f \cdot \boldsymbol{u}_f^*) \, . \tag{A.9}$$

- Join each of these edges as before, though now they will form a closed polygon.

The result is a closed polygon of N segments, still with a beta distribution on segment lengths.

Reference

1. J. Cantarella, T. Deguchi, C. Shonkwiler, Probability theory of random polygons from the quaternionic viewpoint. Commun. Pur. Appl. Anal. **67**, 1658–1699 (2014)