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ABSTRACT

Free motion on a 3-sphere, properly projected on the 2-dimensional manifold of a disk, yields the Zernike system, which exhibits the fundamental properties of superintegrability. These include separability in a variety of coordinate systems, polynomial solutions, and a particular subset of Clebsch-Gordan coefficients as interbasis expansion coefficients that are higher orthogonal polynomials from the Askey scheme. Deriving these results from the initial formulation in spherical geometry provides the Zernike system with interest beyond its optical applications.

I. INTRODUCTION

In our recent research on the Zernike system,[1] we found that the plane disk of a circular pupil where polynomial solutions are sought, when "lifted" to a half-sphere, provides a very clear selection of coordinates where the two dimensions separate the defining Hamiltonian-type differential equation into two such one-dimensional equations. In Ref. 2, we considered three separating coordinate systems, shown in Fig. 1, and all stemming from polar coordinates on the upper half of a 2-sphere $\mathcal{S}^2_+$, whose coordinate poles lie in the z-, x-, and y-directions of the ambient 3-space $\mathcal{R}^3$; they were characterized as systems I, II, and III, respectively. These will be given explicitly in Secs. II–IV. Note that although we also considered *elliptic* coordinate systems,[3,4] those will not be addressed here. The separated solutions for systems I, II, and III involve Legendre, Gegenbauer, and special Jacobi polynomials (and in system I, also a circular trigonometric factor is involved). All these solutions are characterized, by definition, as having finite values at their geometrical boundaries.

On the disk, system I represents the usual *polar* plane coordinate mesh, and Zernike's solutions are characterized by a "principal quantum number" $n \in \mathcal{Z}^+_0 = \{0, 1, 2, \ldots\}$ and "angular momentum" $m \in \{n, n-2, \ldots, -n\}$. Systems II and III, on the other hand, classify the solutions by two indices $n_1, n_2 \in \mathcal{Z}^+_0$ such that $n_1 + n_2 = n$ yields the same principal eigenvalue in the Zernike system; we shall refer to the latter as *Cartesian* coordinate meshes on the disk. Although there is an apparent analogy with the quantum indices in the two-dimensional quantum oscillator on the full plane $\mathcal{R}^2$, its underlying symmetry is a Lie algebra, while the Zernike system leads to a nonlinear Higgs algebra.[2,5]

In Ref. 6, we inquired into the overlap coefficients between solutions in systems I, II, and III. Since the three systems are related through rotations of the full sphere $\mathcal{S}^2$, one could expect that the Wigner SO(3) rotation matrices would play a role. This is not so. The overlap coefficients between the polar- and Cartesian-mesh systems I and II, (n, m) and (n_1, n_2), respectively, turn out to be a special type of *Clebsch-Gordan coefficient*, $C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m}$. These can also be written in analytic form as ${}_3F_2(\cdots|1)$ hypergeometric functions that are particular Hahn polynomials. Previous works by Zernike, Brinkman,[7] and Tango[8] have addressed some of these issues that we discuss at the end of this paper. The connection between the Zernike system and the 3-sphere is here explicitly exploited to yield the wavefunctions, their separating coordinate systems, and thus the Clebsch-Gordan coefficients, as properties of a system that is superintegrable.[10–12]

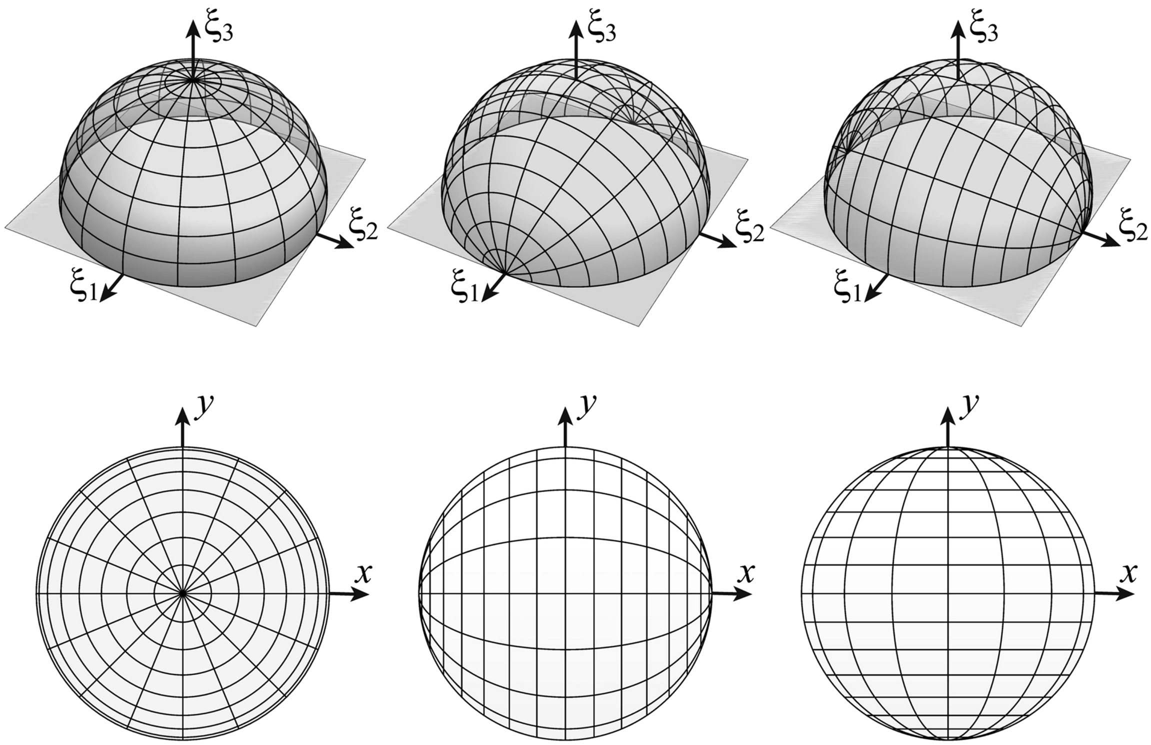

FIG. 1. Top row: three coordinate systems on the upper half-sphere $\vec{\xi} \in \mathcal{S}^2_+$, $|\vec{\xi}| = 1$, and $\xi_3 \geq 0$, referred to as systems I, II, and III. Bottom row: projections of the latter on the disk of the Zernike pupil $\mathbf{r} = (x, y) \in \mathcal{D} \subset \mathcal{R}^2$, $|\mathbf{r}| \leq 1$.

In this paper, we shall elucidate the symmetries behind the appearance of polynomial solutions, by lifting our considerations to the 3-sphere $\mathcal{S}^3$ in an ambient 4-space. The 3-sphere $\mathcal{S}^3$ exhibits six coordinate systems where the Laplace-Beltrami operator separates, and these were found and described in Ref. 9 in the context of quantum free motion in this manifold. In Sec. II, we detail the cylindrical and two spherical coordinate systems of the 3-sphere to be used here, giving the solutions of the Laplace-Beltrami operator that are the complete and orthogonal sets of hyperspherical harmonics.

In Sec. III, we project coordinates of $\mathcal{S}^3$ on the polar and Cartesian coordinates of a 2-dimensional manifold, the upper hemisphere $\mathcal{S}^2_+$. Then, we recall the original differential equation which determines the Zernike system on the domain of the unit circular pupil $\mathcal{D}$, obtained from a vertical projection of the upper half of $\mathcal{S}^2$ shown in Fig. 1, which is itself a projection of the 3-sphere $\mathcal{S}^3$.

In Sec. IV, we bind the hyperspherical harmonics on $\mathcal{S}^3$ to the solutions found in Ref. 2 for the three coordinate systems of $\mathcal{S}^2$. These solutions are so(3) bases for unitary irreducible representations, where the overlap between eigenstates in systems I and II is recognized as representation couplings and given by particular Clebsch-Gordan coefficients, derived in Refs. 6 and 17 through laborious integration. We also generalize system II to system II(α) that are rotated by α from II, which includes system III for $\alpha = \frac{1}{2}\pi$ that results in special Racah polynomials.[6]

As we indicate in Sec. V, referring to the previous works in Refs. 1, 7, and 8, we suggest that a wider endeavor to understand the common origin of a system from free motion on a higher manifold projected in various forms on a compact domain could be fruitful for other two- or higher-dimensional superintegrable systems.

II. COORDINATE SYSTEMS ON THE 3-SPHERE $\mathcal{S}^3$

Before presenting the Zernike system through its differential equation and domain,[1] we dedicate this section to set up the three coordinate systems of the 3-sphere that will be used below to embed this equation.

Consider an ambient 4-space $(s_1, s_2, s_3, s_4) \in \mathcal{R}^4$, embedding the $\mathcal{S}^3$ sphere on the 3-dimensional submanifold Ω_3, determined by $\sum_{i=1}^4 s_i^2 = 1$. In Refs. 9 and 13, its six orthogonal coordinate systems were characterized and called spherical, cylindrical, spheroelliptic, oblate and prolate elliptic, and ellipsoidal. Of these, we need here only the spherical (in two versions) and the cylindrical. Thus, we introduce the following three coordinate sets, with their labels referred to Fig. 1 on $\mathcal{S}^2$, but here preceded by "$\mathcal{S}^3$" to indicate that they parameterize the 3-sphere,

$$\begin{array}{lll}
\textbf{System } \mathcal{S}^3-\textbf{I} & \textbf{System } \mathcal{S}^3-\textbf{II} & \textbf{System } \mathcal{S}^3-\textbf{III} \\
\text{cylindrical:} & \textit{canonical}\text{ spherical:} & \textit{non}-\text{canonical spherical:} \\
s_1=\cos\gamma\cos\phi_1, & s_1=\sin\chi\sin\theta\cos\phi, & s_1=\sin\chi'\cos\theta'\cos\phi', \\
s_2=\cos\gamma\sin\phi_1, & s_2=\sin\chi\sin\theta\sin\phi, & s_2=\sin\chi'\cos\theta'\sin\phi', \\
s_3=\sin\gamma\cos\phi_2, & s_3=\sin\chi\cos\theta, & s_3=\cos\chi', \\
s_4=\sin\gamma\sin\phi_2, & s_4=\cos\chi, & s_4=\sin\chi'\sin\theta', \\
0<\gamma<\tfrac{1}{2}\pi, & 0<\theta,\chi<\pi, & 0<\theta',\chi'<\pi, \\
0\le\phi_1,\phi_2<2\pi. & 0\le\phi<2\pi. & 0\le\phi'<2\pi.
\end{array} \tag{1}$$

To describe the hyperspherical harmonics on the 3-sphere, find conserved quantities, and determine the Clebsch-Gordan coupling coefficients, we recall the construction of the Laplace-Beltrami operator from the six generators of rotations of $\mathcal{S}^3$,

$$L_i := s_j\frac{\partial}{\partial s_k} - s_k\frac{\partial}{\partial s_j}, \qquad M_i := s_i\frac{\partial}{\partial s_4} - s_4\frac{\partial}{\partial s_i} \tag{2}$$

for i,j,k cyclic in $\{1,2,3\}$. These operators close under commutation into the four-dimensional orthogonal Lie algebra $\mathfrak{so}(4)$, namely,

$$[L_i,L_j] = -L_k, \quad [M_i,M_j] = -L_k, \quad [L_i,M_j] = -M_k. \tag{3}$$

The *canonical* subalgebra chain[14] is $\mathfrak{so}(4)\supset\mathfrak{so}(3)\supset\mathfrak{so}(2)$, generated by the operator sets $\{L_i,M_j\}\supset\{L_i\}\supset\{L_3\}$, where the middle set is characterized by the $\mathfrak{so}(3)$ invariant $L^2 := \sum_{i=1}^3 L_i^2$ whose spectrum is well known to be $\ell(\ell+1)$, $\ell\in\mathcal{Z}_0^+$.

The structure of the $\mathfrak{so}(4)$ algebra is further revealed through introducing

$$J_i^{(1)} := \frac{1}{2}(L_i+M_i), \qquad J_i^{(2)} := \frac{1}{2}(L_i-M_i) \tag{4}$$

for $i\in\{1,2,3\}$ and noting that these two sets commute

$$[J_i^{(1)},J_j^{(1)}] = -J_k^{(1)}, \quad [J_i^{(2)},J_j^{(2)}] = -J_k^{(2)}, \quad [J_i^{(1)},J_j^{(2)}] = 0; \tag{5}$$

this algebra *splits* reducing as $\mathfrak{so}(4)=\mathfrak{so}(3)^{(1)}\oplus\mathfrak{so}(3)^{(2)}\supset\mathfrak{so}(2)^{(1)}\oplus\mathfrak{so}(2)^{(2)}$, and where the algebra is now characterized by the two $\mathfrak{so}(3)$ invariants $J^{(1,2)\,2} := \sum_{i=1}^3 (J_i^{(1,2)})^2$, with independent spectra $j^{(1,2)}(j^{(1,2)}+1)$, $j^{(1,2)}\in\mathcal{Z}_0^+$.

Writing $L := (L_1,L_2,L_3)$ and $M := (M_1,M_2,M_3)$, the Lie algebra $\mathfrak{so}(4)$ is seen to have two second-degree invariant Casimir operators, the first of which is L^2+M^2, with spectrum $J(J+2)$, $J\in\mathcal{Z}_0^+$ on $\mathcal{S}^3$, while the second is $L.M+M.L=0$; the latter vanishes because the group coset space on which the algebra acts,[15] i.e., the *realization* of the algebra in the form (2) is on the *group coset* manifold $\Omega_3=\mathrm{SO}(4)/\mathrm{SO}(3)$. This vanishing implies that

$$J^{(1)\,2} = \frac{1}{4}(L\pm M)^2 = J^{(2)\,2} \quad\Rightarrow\quad j^{(1)} = j^{(2)} =: j. \tag{6}$$

The first Casimir operator is the three-dimensional Laplace-Beltrami operator; from whose form and spectrum, we conclude that

$$\left.\begin{array}{llll}
\Delta_{\mathrm{LB}}^{(3)} & := L^2+M^2 & \text{spectrum} & J(J+2) \\
 & = 4J^{(1)\,2} = 4J^{(2)\,2} & \quad '' & 4j(j+1)
\end{array}\right\} \Rightarrow J = 2j\in\mathcal{Z}_0^+. \tag{7}$$

The key properties of this construction are well known: spherical harmonics form eigenspaces of the Laplace-Beltrami operator, which have the discrete, lower-bound spectrum in (7),

$$\Delta_{\mathrm{LB}}^{(3)}\Phi_J(\Omega_3) = -J(J+2)\Phi_J(\Omega_3), \tag{8}$$

and which provides J as a label to classify eigenspaces of solutions. It is also clear that Eq. (8) is independent of the parameterization of Ω_3 and that their differential equations will be different between the three 3-sphere coordinate systems (1).

A. System $\mathcal{S}^3$-I

The cylindrical coordinates of this system in (1) follow the *cylindrical* subalgebra chain $\mathrm{so}(4) = \mathrm{so}(3)^{(1)} \oplus \mathrm{so}(3)^{(2)}$ leading to

$$\Delta_{\mathrm{LB}}^{(3)\,\mathrm{I}} = \frac{\partial^2}{\partial\gamma^2} + (\cot\gamma - \tan\gamma)\frac{\partial}{\partial\gamma} + \frac{1}{\cos^2\gamma}\frac{\partial^2}{\partial\phi_1^2} + \frac{1}{\sin^2\gamma}\frac{\partial^2}{\partial\phi_2^2}. \tag{9}$$

This allows the separation of the solutions $\Phi_J(\gamma,\phi_1,\phi_2)$ and the generators in $\mathrm{so}(2)^{(1)} \oplus \mathrm{so}(2)^{(2)}$; these determine the rest of the quantum number labels,

$$L_3\Phi_{J,m_1,m_2} = \mathrm{i}m_1\Phi_{J,m_1,m_2}, \quad M_3\Phi_{J,m_1,m_2} = \mathrm{i}m_2\Phi_{J,m_1,m_2}. \tag{10}$$

When the explicit form of (9) and that of the generators as differential operators is written out, they lead to a Pöschl-Teller quantum mechanical equation in the angle γ and give J its quadratic spectrum. The (not normalized) solutions to (10) are

$$\begin{aligned}\Phi^{\mathrm{I}}_{J,m_1,m_2}(\gamma,\phi_1,\phi_2) &= (\cos\gamma)^{|m_1|}(\sin\gamma)^{|m_2|}\,P^{(|m_2|,|m_1|)}_{\frac{1}{2}(J-|m_1|-|m_2|)}(\cos 2\gamma)\\ &\times e^{\mathrm{i}(m_1\phi_1+m_2\phi_2)} =: e^{\mathrm{i}m_1\phi_1}\,\Xi^{\mathrm{I}}_{J,m_1,m_2}(\gamma,\phi_2),\end{aligned} \tag{11}$$

labeled by m_1, m_2, being restricted by $J - |m_1| - |m_2| =$ even, and taking special care of their signs. Here, $P_n^{(\alpha,\beta)}(x)$ is a Jacobi polynomial, and Ξ_{J,m_1,m_2} is a function of two angles on $\mathcal{S}^2$.

B. System $\mathcal{S}^3$-II

The canonical spherical coordinates in (1) follow the canonical subalgebra chain $\mathrm{so}(4) \supset \mathrm{so}(3) \supset \mathrm{so}(2)$ and lead to

$$\Delta_{\mathrm{LB}}^{(3)\,\mathrm{II}} = \frac{\partial^2}{\partial\chi^2} + 2\cot\chi\frac{\partial}{\partial\chi} + \frac{1}{\sin^2\chi}\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right), \tag{12}$$

which, in this case, separates $\Phi_J(\chi,\theta,\phi)$ with a different subalgebra chain for the remaining quantum numbers,

$$L^2\Phi_{J,\ell,m} = -\ell(\ell+1)\Phi_{J,\ell,m}, \quad L_3\Phi_{J,\ell,m} = \mathrm{i}m\Phi_{J,\ell,m}, \tag{13}$$

where the branching rules of the orthogonal algebras[14] restrict $0 \le \ell \le J$ and $|m| \le \ell$, all in $\mathcal{Z}_0^+$. The differential Eq. (12) provides us with the (not normalized) solutions,

$$\begin{aligned}\Phi^{\mathrm{II}}_{J,\ell,m}(\chi,\theta,\phi) &= (\sin\chi)^{\ell}\,C^{\ell+1}_{J-\ell}(\cos\chi)\\ &\times P^m_\ell(\cos\theta)e^{\mathrm{i}m\phi} =: e^{\mathrm{i}m\phi}\,\Xi^{\mathrm{II}}_{J,\ell,m}(\chi,\theta),\end{aligned} \tag{14}$$

where $C_n^k(x)$ is a Gegenbauer polynomial and $P_\ell^m(x)$ an associated Legendre polynomial, both satisfying Pöschl-Teller type equations in χ and θ; again $\Xi^{\mathrm{II}}_{J,\ell,m}$ is a function of these two angles.

C. System $\mathcal{S}^3$-III

The *non*canonical spherical coordinates relate to the $\mathcal{S}^3$-II canonical ones through a rotation in the plane of the last two axes, $(s_3,s_4)^{\mathrm{II}} \to (-s_4,s_3)^{\mathrm{III}}$. The subalgebra chain is also $\mathrm{so}(4) \supset \mathrm{so}(3)' \supset \mathrm{so}(2)$ but with a subalgebra $\mathrm{so}(3)'$ rotated in the (s_3,s_4)-plane from the $\mathrm{so}(3)$ subalgebra of $\mathcal{S}^3$-II. This is produced by $\exp(\mathrm{i}\alpha[M_3,\circ])$ for $\alpha = \frac{1}{2}\pi$, mapping $(L_1,L_2) \to (-M_2,M_1)$ and $(M_1,M_2) \to (-L_2,L_1)$, while L_3 and M_3 are invariant. The quadratic operators thus exchange as $L_1^2 + L_2^2 \leftrightarrow M_1^2 + M_2^2$. In the coordinates (1), this entails $\theta \leftrightarrow \theta' + \frac{1}{2}\pi$ so that the canonical Laplace Beltrami operator (12) becomes

$$\Delta_{\mathrm{LB}}^{(3)\,\mathrm{III}} = \frac{\partial^2}{\partial\chi'^2} + 2\cot\chi'\frac{\partial}{\partial\chi'} + \frac{1}{\sin^2\chi'}\left(\frac{\partial^2}{\partial\theta'^2} - \tan\theta'\frac{\partial}{\partial\theta'} + \frac{1}{\cos^2\theta'}\frac{\partial^2}{\partial\phi'^2}\right). \tag{15}$$

This case separates the solutions $\Phi_J^{\mathrm{III}}(\chi',\theta',\phi')$ in the rotated subalgebra chain, cf. (13), namely,

$$(M_1^2+M_2^2+L_3^2)\Phi^{\rm III}_{J,\ell,m} = -\ell'(\ell'+1)\Phi^{\rm III}_{J,\ell',m}, \quad L_3\Phi^{\rm III}_{J,\ell',m} = {\rm i}m\Phi^{\rm III}_{J,\ell',m}, \tag{16}$$

where also in Ref. 14 $0 \le \ell' \le J$ and $|m| \le \ell'$, with the same restrictions and satisfying Pöschl-Teller equations as in the previous system. The (not normalized) solutions of (15) are now, cf. (14),

$$\begin{aligned}\Phi^{\rm III}_{J,\ell',m}(\chi',\theta',\phi') = (\sin\chi')^{\ell'}\, C^{\ell'+1}_{J-\ell'}(\cos\chi') \\ \times P^m_{\ell'}(\sin\theta')e^{{\rm i}m\phi'} =: e^{{\rm i}m\phi'}\,\Xi^{\rm III}_{J,\ell',m}(\chi',\theta').\end{aligned} \tag{17}$$

We have thus three sets of functions of the 3-sphere manifold, each labeled by $J \in \mathcal{Z}_0^+$, and two extra labels stemming from the different subalgebra chains for each coordinate system of $\mathcal{S}^3$. The algebraic problem of relating them has been solved in quantum angular momentum theory and involves the well-known Clebsch-Gordan coefficients.[16] Before applying these results, we should first relate the previous functions on Ω_3 with those on the manifold Ω_2, whose two coordinates are such that one of them has a constant value on the maximal circle that separates the two half-spheres so that the two have independent ranges on the upper 2-sphere, $\mathcal{S}^2_+$ in Fig. 1; this further reduces the three eigenvalue labels in Eqs. (10), (13), and (16) to two.

III. FROM $\mathcal{S}^3$ TO $\mathcal{S}^2$ AND THE ZERNIKE DISK

By means of a useful reparameterization of $\mathcal{S}^3$, we now connect this manifold to the upper-half 2-spheres $\mathcal{S}^2_+$ shown in Fig. 1 that are relevant in the Zernike system and an angle that will be rendered ignorable.

Consider the change of coordinates $(s_1,s_2,s_3,s_4) \mapsto (\xi_1,\xi_2,\xi_3,\varphi)$, where the 3-sphere $\sum_{i=1}^4 s_i^2 = 1$ maps on the 2-sphere $\sum_{i=1}^3 \xi_i^2 = 1$ and $\varphi \in \mathcal{S}^1$ (the circle) given by

$$s_1 = \xi_3\cos\varphi, \quad s_2 = \xi_3\sin\varphi, \quad s_3 = \xi_2, \quad s_4 = \xi_1. \tag{18}$$

In these coordinates, the summands in the Laplace-Beltrami operator $\Delta^{(3)}_{\rm LB}$ contain the two-dimensional $\Delta^{(2)}_{\rm LB}$ in s_3 and s_4, i.e., in (ξ_1,ξ_2,ξ_3), plus derivatives in ξ_3 and φ, thus,

$$\Delta^{(3)}_{\rm LB} = \Delta^{(2)}_{\rm LB} - \sum_{i=1}^3 \xi_i\frac{\partial}{\partial\xi_i} + \frac{1}{\xi_3}\frac{\partial}{\partial\xi_3} + \frac{1}{\xi_3^2}\frac{\partial^2}{\partial\varphi^2}. \tag{19}$$

The application of this operator $\Delta^{(3)}_{\rm LB}$ on the three functions of the 3-sphere, (11), (14), and (17), now applies to functions in the new coordinates (ξ_i,φ), where $\xi_1^2+\xi_2^2+\xi_3^2=1$; this eliminates the term $\sum_{i=1}^3\xi_i\partial_{\xi_i}$ from (19). As we saw, those three functions that we encompass writing them as $\Phi_{J,\nu,\mu}(\vec\xi,\varphi)$ factor into a phase $\exp({\rm i}\mu\varphi)$, time functions on the 2-sphere that we call $\Xi_{J,\nu,\mu}(\vec\xi\,)$, leaving the correspondence between J,ν,μ and the three sub-index sets to be determined below.

With this factorization, we write the solutions (11), (14), and (17) as

$$\Phi_{J,\nu,\mu}(\xi_1,\xi_2,\xi_3,\varphi) = e^{{\rm i}\mu\varphi}\,\Xi_{J,\nu,\mu}(\xi_1,\xi_2,\xi_3), \tag{20}$$

while the Laplace-Beltrami Eq. (8) reduces to

$$\begin{aligned}\Delta^{(3)}_{\rm LB}\Phi_{J,\nu,\mu} &= \left(\widehat{Z} + \tfrac{1}{\xi_3^2}\tfrac{\partial^2}{\partial\varphi^2}\right)\Phi_{J,\nu,\mu} \\ &= \left(\widehat{Z} - \tfrac{\mu^2}{\xi_3^2}\right)\Phi_{J,\nu,\mu} = -J(J+2)\Phi_{J,\nu,\mu},\end{aligned} \tag{21}$$

where we introduce the *Zernike* operator

$$\widehat{Z} := \Delta^{(2)}_{\rm LB} + \frac{1}{\xi_3}\frac{\partial}{\partial\xi_3}. \tag{22}$$

In previous papers,[2,6] the Zernike system was characterized through the quantum-type Hamiltonian operator

$$\widehat{Z}(x,y) = \nabla^2 - (\mathbf{r}\cdot\nabla)^2 - 2\,\mathbf{r}\cdot\nabla, \tag{23}$$

with the domain on the closed unit disk $\mathcal{D} := \{(x,y) \mid x^2+y^2 \le 1\}$ and determining the Schrödinger-type *Zernike* equation,

$$\widehat{Z}(x,y)\,\Psi(\mathbf{r}) = -E\,\Psi(\mathbf{r}), \tag{24}$$

on the space of functions on the disk $\mathcal{D}$ that are *finite* on its boundary,

$$\Psi(\mathbf{r})|_{|\mathbf{r}|=1} < \infty. \tag{25}$$

The eigenfunctions of the Zernike equation (24) with this boundary condition are characterized by the discrete "energy" eigenvalues

$$E = J(J+2), \qquad J \in \mathcal{Z}_0^+. \tag{26}$$

As shown in Ref. 3 for generic elliptic coordinates, and including the three systems in Fig. 1,[4] the solutions (24) are necessarily of polynomial type (in system I, one has also sine and cosine functions). We should emphasize that although the spectrum (26) is identical to the energies of a two-dimensional harmonic oscillator on $\mathcal{R}^2$, the Zernike and oscillator systems are distinct in their Hamiltonians and in their respective boundaries.

The key to finding the symmetry hidden in (23), which is embodied in the separability of its solutions in various coordinate systems, has been to *lift* the unit disk $\mathcal{D}$ to the *upper* half of a 2-sphere $\mathcal{S}_+^2$. This is easily achieved defining new coordinates, purposefully labeled with the same symbols as in (18), and their partial derivatives,

$$\begin{array}{lll} \xi_1 := x, & \xi_2 := y, & \xi_3 := \sqrt{1-x^2-y^2}, \\ \dfrac{\partial}{\partial x} = \dfrac{\partial}{\partial \xi_1} - \dfrac{\xi_1}{\xi_3}\dfrac{\partial}{\partial \xi_3}, & \dfrac{\partial}{\partial y} = \dfrac{\partial}{\partial \xi_2} - \dfrac{\xi_2}{\xi_3}\dfrac{\partial}{\partial \xi_3}. & \end{array} \tag{27}$$

Under this map $(x,y) \in \mathcal{D} \mapsto \vec{\xi} \in \mathcal{S}_+^2$, $|\vec{\xi}| = 1$, and $\xi_3 \geq 0$, the Zernike operator (23) becomes

$$\widehat{Z}(\vec{\xi}) = \Delta_{\text{LB}}^{(2)} - \sum_{i=1}^{3} \xi_i \frac{\partial}{\partial \xi_i} + \frac{1}{\xi_3}\frac{\partial}{\partial \xi_3}, \tag{28}$$

with $\Delta_{\text{LB}}^{(2)}$ being the usual Laplacian on the (ξ_1, ξ_2, ξ_3) surface. When acting on functions independent of $|\vec{\xi}|$ and geometrically fixed to 1, the middle summation term is zero. Hence, we arrive at precisely the Zernike operator in (22). The boundary condition for polynomial solutions, Eq. (25), becomes $\Psi(\xi_1,\xi_2,\xi_3)|_{\xi_3=0} < \infty$.

To establish the bridge between the solutions of the Laplace-Beltrami operator in $\mathcal{S}^3$, $\Phi_{J,\nu,\mu}(\xi_1,\xi_2,\xi_3,\varphi)$ in (20), and solutions $\Psi_{J,\kappa}(\vec{\xi})$ (where κ will stand for ν or μ) of the simple equation on $\mathcal{S}_+^2$,

$$\widehat{Z}(\vec{\xi})\Psi_{J,\kappa}(\vec{\xi}) = \left(\Delta_{\text{LB}}^{(2)} + \frac{1}{\xi_3}\frac{\partial}{\partial \xi_3}\right)\Psi_{J,\kappa}(\vec{\xi}) = -J(J+2)\Psi_{J,\kappa}(\vec{\xi}), \tag{29}$$

clearly the $\mathcal{S}^3$ coordinate $\varphi \in \mathcal{S}^1$ must be made ignorable. This we do next for each of the three coordinate systems.

IV. REDUCTION TO so(3), CLEBSCH-GORDAN COEFFICIENTS AND RACAH POLYNOMIALS

We now render the ignorable phases $\varphi \in \mathcal{S}^1$ in the exponential factors in (11), (14), and (17) by integrating over their circle. This results in a Kronecker δ that sets one of their indices to zero. We refer to the remaining angles to $(x,y) \in \mathcal{D}$ in the disk of the Zernike pupil through (27) for each coordinate system. Thus, we write the (not normalized) solutions as

System I:

$$\begin{aligned} \overline{\Psi}^{\text{I}}_{n,m}(x,y) &:= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi_1\, \Phi^{\text{I}}_{J,m_1,m_2}(\gamma,\phi_1,\phi_2) = \delta_{m_1,0}\Xi^{\text{I}}_{J,0,m_2}(\gamma,\phi_2) \\ &= e^{-\mathrm{i}\frac{1}{2}\pi m}(x^2+y^2)^{\frac{1}{2}|m|}P_{n_r}^{(|m|,0)}\left(1-2(x^2+y^2)\right)e^{\mathrm{i}m\phi}, \end{aligned} \tag{30}$$

$$\begin{aligned} \text{with indices:}\quad & n = J \in \mathcal{Z}_0^+ \text{ principal quant. num.}, \quad m = -m_2, \\ & n_r := \frac{1}{2}(n-|m|) \in \mathcal{Z}_0^+ \textit{ radial} \text{ quantum number}, \\ \text{coordinates:}\quad & x = \xi_1 = \sin\gamma\,\sin\phi_2, \quad y = \xi_2 = \sin\gamma\,\cos\phi_2, \\ & \xi_3 = \cos\gamma, \quad \phi = \frac{1}{2}\pi - \phi_2 \qquad \gamma|_0^{\pi/2},\ \phi|_{-\pi}^{\pi}, \\ \text{eigenfunction of:}\quad & L^2 + M^2 : n(n+2), \quad M_3 : m_2 = -m, \end{aligned} \tag{31}$$

$$\Rightarrow \qquad \Psi^{\text{I}}_{n,m}(x,y) \text{ indices: } n,\ m \in \{-n, -n+2, \ldots, n\}.$$

System II:

$$\bar\Psi^{\text{II}}_{n_1,n_2}(x,y) := \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi\, \Phi^{\text{II}}_{J,\ell,\mu}(\chi,\theta,\phi) = \delta_{\mu,0}\, \Xi^{\text{II}}_{J,\ell,0}(\chi,\theta)$$
$$= (1-x^2)^{\frac{1}{2}n_1} C^{n_1+1}_{n_2}(x)\, P_{n_1}\Big(\frac{y}{\sqrt{1-x^2}}\Big), \tag{32}$$

$$\begin{aligned} \text{with indices: } & n = n_1+n_2 = J \in \mathcal{Z}^+_0 \text{ principal quant. num.}, \ n_1 = \ell, \\ \text{coordinates: } & x = \xi_1 = \cos\chi, \quad y = \xi_2 = \sin\chi\cos\theta, \\ & \xi_3 = \sin\chi\sin\theta, \qquad \chi|_0^\pi,\ \theta|_0^\pi, \\ \text{eigenfunction of: } & L^2+M^2 : n(n+2), \quad L^2 : n_1(n_1+1), \end{aligned} \tag{33}$$

$$\Rightarrow \Psi^{\text{II}}_{n_1,n_2}(x,y) \text{ indices: } n_1 \in \{0,1,\ldots,n\}, \quad n_2 = n-n_1.$$

System III:

$$\bar\Psi^{\text{III}}_{n_1',n_2'}(x,y) := \frac{1}{2\pi}\int_{-\pi}^{\pi} d\phi'\, \Phi^{\text{III}}_{J,\ell',\mu}(\chi',\theta',\phi') = \delta_{\mu,0}\, \Xi^{\text{III}}_{J,\ell',0}(\chi',\theta')$$
$$= (1-y^2)^{\frac{1}{2}n_1'} C^{n_1'+1}_{n_2'}(y)\, P_{n_1'}\Big(\frac{x}{\sqrt{1-y^2}}\Big), \tag{34}$$

$$\begin{aligned} \text{with indices: } & n = n_1'+n_2' = J \in \mathcal{Z}^+_0 \text{ principal quant. num.}, \ n_1' = \ell', \\ \text{coordinates: } & x = \xi_1 = \sin\chi'\sin\theta', \quad y = \xi_2 = \cos\chi', \\ & \xi_3 = \sin\chi'\cos\theta', \qquad \chi'|_0^\pi,\ \theta'|_{-\pi/2}^{\pi/2}, \\ \text{eigenfunction of: } & L^2+M^2 : n(n+2), \quad M_1^2+M_2^2+L_3^2 : n_1'(n_1'+1), \end{aligned} \tag{35}$$

$$\Rightarrow \Psi^{\text{II}}_{n_1',n_2'}(x,y) \text{ indices: } n_1' \in \{0,1,\ldots,n\}, \quad n_2' = n-n_1'.$$

Here, $P_n^{(\alpha,\beta)}(x)$, $C_n^m(x)$, and $P_n(x)$ are Jacobi, Gegenbauer, and Legendre polynomials, respectively.

A. States in system I

With this list, let us now return to the algebraic structure of $\mathrm{so}(4)$ seen in Sec. II to identify system I with its subalgebra chain $\mathrm{so}(4) = \mathrm{so}(3)^{(1)} \oplus \mathrm{so}(3)^{(2)}$ through defining $J^{(1,2)}$ in (4) and (5). Recall Eq. (7), where we concluded that their two $\mathrm{so}(3)$ Casimir operators $J^{(1,2)2}$ characterize these representations by $j^{(1,2)} = \frac{1}{2}J = \frac{1}{2}n$. We also recall that as Lie *group manifolds*, one has $\mathrm{SO}(4) = \mathrm{SU}(2)^{(1)} \otimes \mathrm{SU}(2)^{(2)}$, so the functions on the 3-sphere can beget two-valued functions on the real 2-sphere.

Regarding the $\mathrm{so}(3)$ representation row eigenlabel $-m$ of M_3 in (31), we note that $M_3 = J_3^{(1)} - J_3^{(2)}$ so that the $J_3^{(1,2)}$ eigenlabels will be such that $m^{(1)} - m^{(2)} = -m$. Yet looking back at (2), we see that L_3 rotates the (s_1,s_2)-plane which, according to (18), is over the angle φ that was integrated in (30) so that L_3 is projected to zero; hence, $J_3^{(1)} = -J_3^{(2)}$ and $m^{(1)} = -m^{(2)}$. The row labels in this subalgebra chain are therefore $m^{(1)} = -\frac{1}{2}m$ and $m^{(2)} = \frac{1}{2}m$. In a convenient bra-ket notation, we can thus write the (normalized) solutions in system I coordinates as

$$\Psi^{\text{I}}_{n,m}(x,y) = C^{\text{I}}_{n,m}\overline{\Psi}^{\text{I}}_{n,m}(x,y) = \Big(x,y\,\Big|\,\frac{1}{2}n,\ -\frac{1}{2}m\Big\rangle^{\text{I}}\Big|\,\frac{1}{2}n,\ \frac{1}{2}m\Big\rangle^{\text{I}}, \tag{36}$$

where $|x,y)$ with $(x,y)\in\mathcal{D}$ is the Dirac basis for functions on the disk. Up to a phase $\omega^{\text{I}}_{n,m}$, the normalization constant $C_{n,m}$ is equal to[2]

$$C^{\mathrm{I}}_{n,m} = \omega^{\mathrm{I}}_{n,m}(-1)^{n_r}\sqrt{(n+1)/\pi}. \tag{37}$$

B. States in system II

System II is based on the canonical Gel'fand-Zetlin subalgebra chain $\mathrm{SO}(4) \supset \mathrm{SO}(3) \supset \mathrm{SO}(2)$, here in representations where $L.M + M.L = 0$ and reduced by $L_3 = 0$ as in system I; the SO(4) eigenstates $|J, \ell, m\rangle$ are, according to (33), labeled $|n, n_1, 0\rangle$ and SO(3) states $|n_1, 0\rangle^{\mathrm{II}}$. Thus, as in (36) and $n_1 + n_2 = n$,

$$\Psi^{\mathrm{II}}_{n_1,n_2}(x,y) = C^{\mathrm{II}}_{n_1,n_2}\overline{\Psi}^{\mathrm{II}}_{n_1,n_2}(x,y) = (x,y\,|\,n_1,0\rangle^{\mathrm{II}}, \tag{38}$$

and, up to a phase $\omega^{\mathrm{II}}_{n_1,n_2}$, the normalization constant is[2]

$$C^{\mathrm{II}}_{n_1,n_2} := \omega^{\mathrm{II}}_{n_1,n_2} 2^{n_1+\frac{1}{2}} n_1! \sqrt{\frac{(2n_1+1)(n_1+n_2+1)\,n_2!}{2\pi\,(2n_1+n_2+1)!}}. \tag{39}$$

Finally, it can be seen that system III is only a $\frac{1}{2}\pi$-rotation of the (x,y) disk to $(y,-x)$ of system II, so the above results are valid replacing n_i by n_i', picking up an extra phase. The II–III interbasis expansion will be discussed after examining further the I–II expansion.

C. Interbasis expansion I–II

Having written $\Psi^{\mathrm{I}}_{n,m}(x,y)$ and $\Psi^{\mathrm{II}}_{n_1,n_2}(x,y)$ as SO(3) states, we inquire into the direct and inverse expansions

$$\Psi^{\mathrm{II}}_{n_1,n_2}(x,y) = \sum_{m=-n\,(2)}^{n} W^{n,m}_{n_1,n_2}\,\Psi^{\mathrm{I}}_{n,m}(x,y), \tag{40}$$

$$\Psi^{\mathrm{I}}_{n,m}(x,y) = \sum_{n_1=0}^{n} \tilde{W}^{n_1,n_2}_{n,m}\,\Psi^{\mathrm{II}}_{n_1,n_2}(x,y), \tag{41}$$

where $n_2 = n - n_1$ and $\sum_{m=-n\,(2)}^{n}$ indicates that $m \in \{-n, -n+2, \ldots, n\}$. Using (36) and (38), we write (40) in bra-ket form as

$$(x,y|n_1,0\rangle^{\mathrm{II}} = (x,y|\sum_{m=-n\,(2)}^{n} |\tfrac{1}{2}n, -\tfrac{1}{2}m\rangle^{\mathrm{I}} |\tfrac{1}{2}n, \tfrac{1}{2}m\rangle^{\mathrm{I}}\; {}^{\mathrm{I}}\langle\tfrac{1}{2}n, \tfrac{1}{2}m| {}^{\mathrm{I}}\langle\tfrac{1}{2}n, -\tfrac{1}{2}m|n_1,0\rangle^{\mathrm{II}}. \tag{42}$$

We thus recognize that the linear combination coefficients in (40) are, up to phases ω, a special subset of Clebsch-Gordan coefficients,

$$W^{n,m}_{n_1,n_2} = {}^{\mathrm{I}}\langle\tfrac{1}{2}n, \tfrac{1}{2}m|\, {}^{\mathrm{I}}\langle\tfrac{1}{2}n, -\tfrac{1}{2}m|n_1,0\rangle^{\mathrm{II}} = \omega\, C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m} = \widetilde{W}^{n_1,n_2\,*}_{n,m}, \tag{43}$$

where the asterisk indicates complex conjugation.

It is useful to recall that the general form of the Clebsch-Gordan coefficients, $C^{j,m}_{j_1,m_1;j_2,m_2}$, couples the SO(3) states $|j_1, m_1\rangle$ and $|j_2, m_2\rangle$ to a single state $|j, m\rangle$ with the usual branching rules $|j_1 - j_2| \le j \le j_1 + j_2$ and $m_1 + m_2 = m$. A property of the special kind of coefficient (43) is that, as shown in Ref. 6, they can be written in terms of hypergeometric ${}_3F_2(\cdots|1)$ terminating series which are known as Hahn polynomials,

$$C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m} = \frac{n!}{\left(\frac{1}{2}(n_1-n_2-m)\right)!\left(\frac{1}{2}(n+m)\right)!}\sqrt{\frac{2n_1+1}{n_2!\,(n+n_1+1)!}} \times {}_3F_2\left(\begin{matrix}-n_2, & n_1+1, & -\frac{1}{2}(n+m)\\ -n, & \frac{1}{2}(n_1-n_2-m)+1 & \end{matrix}\middle|\,1\right) \tag{44}$$

$$= \frac{(n!)^2}{\left(\frac{1}{2}(n-m)\right)!\left(\frac{1}{2}(n+m)\right)!}\sqrt{\frac{2n_1+1}{n_2!\,(n+n_1+1)!}} \times Q_{n_2}\left(\frac{1}{2}(n+m);\, -n-1,\, -n-1,\, n\right). \tag{45}$$

Wenote that of the five parameters available in ${}_3F_2(\cdots|1)$ and in $Q.(.;.,.,.)$, only three, e.g., (n_1, n_2, m), are present in the interbasis coefficients $W^{n,m}_{n_1,n_2}$. Their phase was determined in Ref. 6 through direct integration of pairs of basis functions and is given by

$$W^{n,m}_{n_1,n_2} = \mathrm{i}^{n_1}(-1)^{\frac{1}{2}(m+|m|)}\, C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m}. \tag{46}$$

We should mention that this phase is the appropriate one to intertwine between the complex system I functions $\Psi^{\mathrm{I}}_{n,m}(x,y)^* = \Psi^{\mathrm{I}}_{n,-m}(x,y)$ and the real system II functions $\Psi^{\mathrm{II}}_{n_1,n_2}(x,y)$, which is assured by the property $C^{n_1,0}_{\frac{1}{2}n,\frac{1}{2}m;\,\frac{1}{2}n,-\frac{1}{2}m} = (-1)^{n_2} C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m}$.

D. Interbasis expansions I–III

We now turn to system III, which we saw is obtained from system II by the rotation $(x,y)\mapsto(y,-x)$ of the disk plane and is generated by M_3 through $\widehat{R}(\alpha) := \exp(\mathrm{i}\alpha[M_3,\circ])$ for $\alpha = \frac{1}{2}\pi$. Keeping $\alpha\in\mathcal{S}^1$ generic, we can thus define systems II(α), all of whose eigenstates will be characterized by the pair of integers (n_1,n_2) with $n_1+n_2=n$. Since $M_3 = J^{(1)}_3 - J^{(2)}_3$ (as $L_3 = 0$), we have

$$\begin{aligned}\widehat{R}\alpha\left|\frac{1}{2}n,-\frac{1}{2}m\right\rangle^{\mathrm{I}}\left|\frac{1}{2}n,\frac{1}{2}m\right\rangle^{\mathrm{I}} &= e^{\mathrm{i}\alpha J^{(1)}_3}\left|\frac{1}{2}n,-\frac{1}{2}m\right\rangle^{\mathrm{I}} e^{-\mathrm{i}\alpha J^{(2)}_3}\left|\frac{1}{2}n,\frac{1}{2}m\right\rangle^{\mathrm{I}}\\ &= e^{-\mathrm{i}\alpha m}\left|\frac{1}{2}n,-\frac{1}{2}m\right\rangle^{\mathrm{I}}\left|\frac{1}{2}n,\frac{1}{2}m\right\rangle^{\mathrm{I}}.\end{aligned} \tag{47}$$

The expansion of system II(α) solutions in terms of system I basis for the principal quantum number n, analog of (40), is thus

$$\Psi^{\mathrm{II}(\alpha)}_{n_1,n_2}(x,y) = \sum_{m=-n\,(2)}^{n} W^{n,m\,(\alpha)}_{n_1,n_2}\,\Psi^{\mathrm{I}}_{n,m}(x,y), \tag{48}$$

with the coefficients $W^{n,m\,(\alpha)}_{n_1,n_2}$ directly related to $W^{n,m}_{n_1,n_2} = W^{n,m\,(0)}_{n_1,n_2}$ as

$$W^{n,m\,(\alpha)}_{n_1,n_2} = e^{-\mathrm{i}\alpha m}\,W^{n,m\,(0)}_{n_1,n_2} = e^{-\mathrm{i}\alpha m}\,\mathrm{i}^{n_1}(-1)^{\frac{1}{2}(m+|m|)}\,C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m}. \tag{49}$$

The inverse transformation (41) from system II(α) to I is now

$$\Psi^{\mathrm{I}}_{n,m}(x,y) = \sum_{n_1=0}^{n}\widetilde{W}^{n_1,n_2}_{n,m\,(\alpha)}\,\Psi^{\mathrm{II}(\alpha)}_{n_1,n_2}(x,y), \tag{50}$$

with

$$\widetilde{W}^{n_1,n_2}_{n,m\,(\alpha)} = e^{\mathrm{i}m\alpha}\,\widetilde{W}^{n_1,n_2}_{n,m\,(0)} = W^{n,m\,(\alpha)*}_{n_1,n_2}. \tag{51}$$

Clearly, for $\alpha = \frac{1}{2}\pi$, we are addressing system III as written in Ref. 6, up to a possible overall phase.

We can now formulate the transformation between states in systems II(α) and II(β) by passing through system I,

$$\begin{aligned}\Psi^{\mathrm{II}(\beta)}_{n'_1,n'_2}(x,y) &= \sum_{m=-n\,(2)}^{n} W^{n,m\,(\beta)}_{n'_1,n'_2}\sum_{n_1=0}^{n}\widetilde{W}^{n_1,n_2}_{n,m\,(\alpha)}\,\Psi^{\mathrm{II}(\alpha)}_{n_1,n_2}(x,y)\\ &= \sum_{n_2=0}^{n} U^{n_1,n_2}_{n'_1,n'_2}(\beta-\alpha)\,\Psi^{\mathrm{II}(\alpha)}_{n_1,n_2}(x,y),\end{aligned} \tag{52}$$

where the compound transformation coefficients are

$$\begin{aligned}U^{n_1,n_2}_{n'_1,n'_2}(\gamma) &:= e^{\mathrm{i}\frac{1}{2}\pi(n'_1-n_1)}\sum_{m=-n\,(2)}^{n} e^{-\mathrm{i}\gamma m}\,C^{n'_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m}\,C^{n_1,0}_{\frac{1}{2}n,-\frac{1}{2}m;\,\frac{1}{2}n,\frac{1}{2}m}\\ &= e^{\mathrm{i}(n\gamma+\frac{1}{2}\pi(n'_1-n_1))}\sum_{k=0}^{n} e^{-2\mathrm{i}\gamma k}\,C^{n'_1,0}_{\frac{1}{2}n,\frac{1}{2}n-k;\,\frac{1}{2}n,-\frac{1}{2}n+k}\,C^{n_1,0}_{\frac{1}{2}n,\frac{1}{2}n-k;\,\frac{1}{2}n,-\frac{1}{2}n+k}.\end{aligned} \tag{53}$$

When the $\Psi^{\mathrm{II}(\beta)}_{n'_1,n'_2}(x,y)$ are arranged into column vectors with components (n_1,n_2), the coefficients $U^{n_1,n_2}_{n'_1,n'_2}(\gamma)$ can be fit into matrices which, for every fixed principal quantum number n, compose as

$$\sum_{n'_1,n'_2} U^{n_1,n_2}_{n'_1,n'_2}(\gamma_1)\,U^{n'_1,n'_2}_{n''_1,n''_2}(\gamma_2) = U^{n_1,n_2}_{n''_1,n''_2}(\gamma_1+\gamma_2). \tag{54}$$

E. The interbasis expansion II–III

When the angle between the two coordinate systems in Subsection IV D is $\gamma = \frac{1}{2}\pi$, the transform kernel (53) takes the form of a special Racah polynomial[6] that relates solutions in systems II and III in Fig. 1. It is of interest to rederive this result using the algebraic properties of the so(4) generators (2)–(5).

Consider the interbasis expansion between the two functions on $\mathcal{S}^3$ sphere, $\Phi^{\rm II}_{J,\ell,m}(\chi,\theta,\phi)$ in (14) and $\Phi^{\rm III}_{J,\ell',m}(\chi',\theta',\phi')$ in (17),

$$\Phi^{\rm III}_{J,\ell',m}(\chi',\theta',\phi') = \sum_{\ell=|m|}^{J} W^{J,|m|}_{\ell',\ell}\Phi^{\rm II}_{J,\ell,m}(\chi,\theta,\phi), \tag{55}$$

where we shall derive recursion relations for these $\mathcal{S}^3$-interbasis coefficients $W^{J,|m|}_{\ell',\ell}$ which form $(J-|m|)\times(J-|m|)$ matrices. Below, when projecting on the $\mathcal{S}^2$-interbasis of Zernike solutions, m becomes 0, while the $W^{J}_{\ell',\ell}$-matrix will split into four submatrices because of parity.

The two $\mathcal{S}^3$-function sets are common eigenfunctions of the Laplace-Beltrami operator $\Delta^{(3)\,\rm II}_{\rm LB}$ in (12) and L_3^2; they are distinguished by their intermediate so(3) subgroup link in so(4), as given by (33) and (35),

$$(L_1^2+L_2^2+L_3^2)\Phi^{\rm II}_{J,\ell,m}(\chi,\theta,\phi) = -\ell(\ell+1)\Phi^{\rm II}_{J,\ell,m}(\chi,\theta,\phi), \tag{56}$$

$$(M_1^2+M_2^2+L_3^2)\Phi^{\rm III}_{J,\ell',m}(\chi',\theta',\phi') = -\ell'(\ell'+1)\Phi^{\rm III}_{J,\ell',m}(\chi',\theta',\phi'), \tag{57}$$

but share a common so(2) subgroup generated by L_3 and the eigenvalue m.

To extract the coefficients $W^{J,|m|}_{\ell',\ell}$ in (55), we note that $M_1^2+M_2^2 = \Delta^{(3)}_{\rm LB} - L^2 - M_3^2$, so we replace (57) into the expansion (55), multiply by $\Phi^{\rm II}_{J,\ell',m}(\chi,\theta,\phi)^*$, and then integrate over the 3-sphere $\mathcal{S}^3$ with the measure $d\omega = \sin^2\chi\,\sin\theta\,d\chi\,d\theta\,d\phi$. We find

$$\sum_{\ell=|m|}^{J} W^{J,|m|}_{\ell',\ell}\Big([\ell'(\ell'+1)+\ell(\ell+1)-J(J+2)]\delta_{\ell'\,\ell} - M^{J,m}_{\ell,\ell'}\Big) = 0, \tag{58}$$

$$\text{where}\qquad M^{J,m}_{\ell',\ell} = \int_{\mathcal{S}^3}\Phi^{\rm II*}_{J,\ell',m}(\chi,\theta,\phi)\,M_3^2\,\Phi^{\rm II}_{J,\ell,m}(\chi,\theta,\phi)\,d\omega. \tag{59}$$

Weuse the explicit form of the so(4) generator M_3 in 3-spherical coordinates,

$$M_3 = -\cos\theta\frac{\partial}{\partial\chi} + \cot\chi\,\sin\theta\frac{\partial}{\partial\theta}, \tag{60}$$

to compute its matrix representation $\mathbf{M}_3^{(J,m)} := \|\mathcal{M}^{J,m}_{\ell',\ell}\|$ in the basis of functions $\Phi^{\rm II}_{J,\ell,m}$, which is bidiagonal, through the integral

$$\begin{aligned}\mathcal{M}^{J,m}_{\ell',\ell} &:= \int_{\mathcal{S}^3}\Phi^{\rm II*}_{J,\ell',m}(\chi,\theta,\phi)\,M_3\,\Phi^{\rm II}_{J,\ell,m}(\chi,\theta,\phi)\,d\omega \\ &= \sqrt{\frac{(\ell-m+1)(\ell+m+1)(J+\ell+2)(J-\ell)}{(2\ell+1)(2\ell+3)}}\;\delta_{\ell',\ell+1} \\ &\quad - \sqrt{\frac{(\ell-m)(\ell+m)(J+\ell+1)(J-\ell+1)}{(2\ell+1)(2\ell-1)}}\;\delta_{\ell',\ell-1}.\end{aligned} \tag{61}$$

Then, we find the tridiagonal matrix of its square, M_3^2 in (59), introducing the usual sum over an orthogonal and complete set of states $\{\phi_k\}$ between a product of two operators A, B as $(\phi_i, AB\phi_j) = \sum_k(\phi_i, A\phi_k)(\phi_k, B\phi_j)$. Thus, we obtain

$$M^{J,m}_{\ell',\ell} = \sum_{\ell''=|m|}^{J}\mathcal{M}^{J,m}_{\ell',\ell''}\mathcal{M}^{J,m}_{\ell'',\ell} = C^{|m|}_{\ell}\delta_{\ell',\ell+2} - E^{|m|}_{\ell}\delta_{\ell',\ell} + C^{|m|}_{\ell-2}\delta_{\ell',\ell-2}, \tag{62}$$

where

$$C_\ell^{|m|} = \sqrt{\frac{(J-\ell-1)(J-\ell)(J+\ell+2)(J+\ell+3)}{(2\ell+1)(2\ell+3)^2(2\ell+5)}} \times\sqrt{(\ell-|m|+1)(\ell-|m|+2)(\ell+|m|+1)(\ell+|m|+2)}, \tag{63}$$

$$E_\ell^{|m|} = \frac{(J-\ell+1)(J+\ell+1)(\ell^2-m^2)}{(2\ell-1)(2\ell+1)} + \frac{(J-\ell)(J+\ell+2)(\ell-|m|+1)(\ell+|m|+1)}{(2\ell+1)(2\ell+3)}. \tag{64}$$

Finally, introducing this expression in (58), we obtain the following three-term recurrence relation for the II-III interbasis coefficients $W^{J,|m|}_{\ell',\ell}$ in (55),

$$C_\ell^{|m|} W^{J,|m|}_{\ell',\ell+2} + \Big(J(J+2) - \ell(\ell+1) - \ell'(\ell'+1) - E_\ell^{|m|}\Big) W^{J,|m|}_{\ell',\ell} + C_{\ell-2}^{|m|} W^{J,|m|}_{\ell',\ell-2} = 0. \tag{65}$$

This recursion relation stems from the integration of (59), where we applied the operator M_3^2 on $\Phi^{\rm II}_{J,\ell,m}$ to its right. However, since this operator is self-adjoint under integration over the 3-sphere, it can be equally applied on $\Phi^{\rm II\,*}_{J,\ell',m}$ to its left. The result is a recursion relation identical to (65) with the exchange $\ell \leftrightarrow \ell'$ for $W^{J,|m|}_{\ell',\ell}$. In addition, observe that (65) is a *2-step* recursion, which can begin for ℓ' and ℓ from $0, 2, \ldots$ or from $1, 2, \ldots$, so we have *four* classes of coefficients for $(\ell', \ell) \in \{(0,0),(0,1),(1,0),(1,1)\}$, determined by their parity under the reflections $\theta' \leftrightarrow -\theta'$ in Eq. (17) and $\theta \leftrightarrow -\theta$ in (14), respectively.

To obtain the $\mathcal{S}^2$ II-III eigenbases expansion between the Zernike functions, which stem from the above 3-sphere expansion (55), we integrate over the angle ϕ; this angle is common to both systems because they share the same generator L_3. We thus integrate (32) and (34), resulting in the L_3 eigenvalue $m = 0$. We can compare this projection of the $\mathrm{so}(4)$ interbasis expansion with the result in Ref. 6,

$$U^{n_1,n_2}_{n_1',n_2'} = W^{J,0}_{n_1,n_1'}, \qquad J = n = n_1 + n_2 = n_1' + n_2'. \tag{66}$$

The recurrence relation (65) for $m = 0$ simplifies somewhat and leads to a 1-step recurrence between terms $p = \frac{1}{2}\ell$ and $p = \frac{1}{2}(\ell+1)$ according to parity and their neighbors $p \pm 1$. This results in four recurrence relations, each of them characterizing Racah polynomials [Ref. 18, Eq. (9.2.3)], $R_p(\lambda(x); \alpha, \beta, \gamma, \delta)$ of degree p, orthogonal on a quadratic lattice $\lambda(x) = x(x+\gamma+\delta+1)$, times a factor that includes the orthogonality measures in x and p, and four effective parameters among the six that are generic. (The explicit values of the parameters and the corresponding Racah polynomials are given in our previous work.[6]) In this way, we have explained the II-III interbasis expansion and its coefficients that overlap between two $\frac{1}{2}\pi$-rotated $\mathrm{so}(3)$ subalgebra chain bases of $\mathrm{so}(4)$ that share the same $\mathrm{so}(2)$ bottom subalgebra, after the reduction through integration over the circle of the latter.

V. CONCLUDING REMARKS

In this paper, we have established the link between hyperspherical harmonics on the 3-sphere, which describe a free quantum system on that manifold, with the polynomial solutions of the Zernike system on the upper-half 2-sphere and thus on the unit disk. The many properties of the former, such as separation of variables and superintegrability, are thus inherited from the former to the latter.[12] The requirement (25) for the Zernike solutions to be finite on the disk boundary is automatically fulfilled since the hyperspherical harmonics is finite over their spheres.

Orthogonal coordinate systems on spheres have been a persistent topic of research, credibly introduced by Olevsky[19] in 1950; thereafter, the hyperspherical harmonic functions on the 3-sphere were related to special Wigner (Clebsch-Gordan) coefficients through $\mathrm{so}(4)$ Lie-algebraic recurrence relations by Stone[20] in 1955. Analytic and algebraic studies of this manifold and group have been pursued by many other authors for 2-, 3-, and n-spheres.[21–23] As we mentioned in the Introduction, there exist six systems of coordinates which allow separation of variables in Helmholtz equation on the 3-sphere, namely, spherical (canonical), cylindrical, two ellipsocylindrical, spheroconical, and ellipsoidal. Four of them, spherical (canonical and noncanonical) cylindrical, and two ellipsocylindrical, conform to Eq. (19). The latter two, leading to Heun polynomial solutions in the Zernike system,[3] have not been examined in this paper, but their $\mathrm{so}(4)$ origin has been applied to separable solutions of the Kepler system, and their expansion coefficients to the two other systems found by Grosche *et al.*[9]

From the side of the physical system, shortly after the Zernike 1934 paper[1] appeared, the differential equation and its solutions were related to the p-dimensional Laplace-Beltrami equation and hyperspherical solutions and products of Gegenbauer polynomials, in a rarely quoted paper of Zernike and Brinkman.[7] For the most part, the Zernike polynomials were analyzed in terms of their recurrence relations and orthogonality properties,[24–29] their efficient computation,[30] and mainly on their applications to the real-time correction of flexible and segmented optical telescopes (see, e.g., Refs. 8 and 31).

By linking the properties of the Zernike system to that of free motion on the 3-sphere through the reduction of $\mathrm{so}(4)$ representations to $\mathrm{so}(3)$ ones and their Clebsch-Gordan couplings, we obtain a unifying view of their common or derivable properties. These include separability, i.e., superintegrability and interbasis expansions. We note that an expanded analysis of the elliptic coordinate system can follow, as well as a corresponding analysis on 3-hyperboloids, where the Lorentz algebra $\mathrm{so}(3,1)$ will be at play.

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