

Hyperspherical harmonics with arbitrary arguments

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The derivation scheme for hyperspherical harmonics (HSH) with arbitrary arguments is proposed. It is demonstrated that HSH can be presented as the product of HSH corresponding to spaces with lower dimensionality multiplied by the orthogonal (Jacobi or Gegenbauer) polynomial. The relation of HSH to quantum few-body problems is discussed. The explicit expressions for orthonormal HSH in spaces with dimensions from two to six are given. The important particular cases of four- and six-dimensional spaces are analyzed in detail and explicit expressions for HSH are given for several choices of hyperangles. In the six-dimensional space, HSH representing the kinetic-energy operator corresponding to (i) the three-body problem in physical space and (ii) four-body planar problem are derived. © 2009 American Institute of Physics. [DOI: 10.1063/1.3054274]

I. INTRODUCTION

The hyperspherical harmonics (HSH) are an important tool in the study of quantum few-body systems. This is caused by the fact that the kinetic-energy operator of an N -particle system is equivalent to the Laplace operator in the space of $3N$ dimensions (or $2N$, in the case of planar systems). The amount of papers in which HSH are applied to specific physical problems is very large. We mention only few recent review articles¹⁻⁴ and a book.⁵

HSH are functions of $d-1$ dimensionless variables (hyperangles) which describe the points on the hypersphere. Of course, the choice of hyperangles is not unique and it is a matter of convenience. The only exception is the three-dimensional (3D) space, where the arguments of the spherical harmonics are conventional spherical angles $\theta = \arccos z / \sqrt{x^2 + y^2 + z^2}$ and $\phi = \arctan x/y$. The generalization of this definition on spaces with $d > 3$ is the following. Let $\mathbf{r} = (x_1, x_2, \dots, x_d)$ be the d -dimensional radius vector, then the hyperspherical angles are defined by the equations,⁶

$$\begin{aligned} x_1 &= R \cos \theta_1, \\ x_2 &= R \sin \theta_1 \cos \theta_2, \\ x_3 &= R \sin \theta_1 \sin \theta_2 \cos \theta_3, \\ &\dots \\ x_{d-1} &= R \sin \theta_1 \dots \sin \theta_{d-2} \cos \phi \\ x_d &= R \sin \theta_1 \dots \sin \theta_{d-2} \sin \phi, \end{aligned} \tag{1}$$

where $\phi \in [0, 2\pi)$, $\theta_\kappa \in [0, \pi]$, and $\kappa = 1, 2, \dots, d-2$.

The J th rank HSH $H_\epsilon^J(\hat{\mathbf{r}})$ is defined by the Laplace equation

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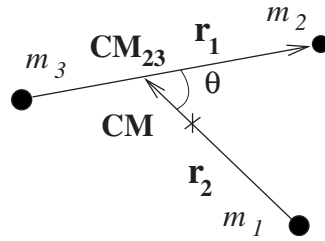


FIG. 1. Jacobi vectors (Ref. 7) for the three-body system. CM_{23} is the center of mass of the pair m_2, m_3 .

$$\Delta r^J H_\epsilon^J(\hat{\mathbf{r}}) = 0, \quad (2)$$

where $\Delta = \sum_{k=1}^d \partial^2 / \partial x_k^2$ and ϵ denotes the set of indices which label different HSH of the same rank.

The explicit expression for HSH depending on the hyperspherical angles (1) is well known [see Eq. (11.2.23) of Ref. 6]. It is given by the product of Gegenbauer (ultraspherical) polynomials, so that k th polynomial in the product depends on $\cos \theta_k$.

However, in many physical applications the set of hyperspherical angles is not convenient. For example, in the quantum three-body problem one has to deal with six-dimensional (6D) vector space being the product of two 3D spaces corresponding to the Jacobi vectors; see Fig. 1. Thus, in this case it is more adequate to parametrize the arguments of HSH by the spherical angles of the 3D vectors $\mathbf{r}_1, \mathbf{r}_2$. Further aspects of the choice of coordinates in the three-body problem including analysis of the permutational symmetry are discussed in Ref. 8.

HSH in $3N$ -dimensional space depending on the spherical angles of N 3D vectors may serve as a convenient basis for the decomposition of the wave function of the quantum many-particle system. The arguments of corresponding HSH comprise, apart from $2N$ 3D spherical angles of vectors $\mathbf{r}_1, \dots, \mathbf{r}_N$, $N-1$ hyperangles which describe the lengths r_1, r_2, \dots, r_N . Again, there is freedom in choice of the hyperangles. For example, one can define the hyperangles similarly to (1) by replacing $x_k \rightarrow r_k$. Such set of the hyperangles was used in Ref. 9, where the explicit expressions for the corresponding HSH have been derived by means of the explicit solution of the Laplace equation.

The physical nature of the problem may suggest different choice of the connection of the hyperangles with the vectors describing the system. Thus, the problem is how to derive the explicit expression for HSH corresponding to various choices of their arguments. The conventional approach,^{6,9,10} consists in the transformation of the Laplacian to the desired hyperangular variables with the subsequent solution of the ensuing partial differential equation. Such approach has been used in Ref. 8 where the number of relations for HSH has been presented using the so-called “method of trees.”

It is desirable to develop the technique of the derivation of HSH which would not require the transformation of the Laplacian. In the presented paper such technique is proposed. It allows one to derive the expressions for HSH depending on an arbitrary set of hyperangles. The technique is based on the concept of zero-length vectors proposed initially by Cartan.^{11,12} The developed calculation scheme is recursive, i.e., HSH in space with higher dimensions is presented as the product of lower-dimensional HSH with some weight function being an orthogonal polynomial. As the examples of the proposed technique, various representations for HSH in spaces with $d = 2, 3, 4, 5, 6$ are derived.

II. THE GENERAL FORMALISM

Below the expression for the scalar product of HSH is derived in Sec. II A. Next, in Sec. II B several general expressions for HSH are derived in terms of lower-rank HSH. The final expressions for normalized HSH and surface elements in d -dimensional space are given in Sec. II C.

A. The scalar product of HSH

It is important that the expression for the scalar product of HSH can be derived without the knowledge of their explicit form. In order to demonstrate this, let us consider the scalar function $f_J(\mathbf{r}, \mathbf{r}')$ defined by

$$f_J(\mathbf{r}, \mathbf{r}') = r^{2J+d-2} (\mathbf{r}' \cdot \nabla)^J \frac{1}{r^{d-2}}, \quad (3)$$

where \mathbf{r}, \mathbf{r}' are d -dimensional vectors. Obviously, f_J is a homogeneous polynomial of degree J with respect to the components of \mathbf{r} or \mathbf{r}' . Namely,

$$f_J(\alpha \mathbf{r}, \beta \mathbf{r}') = (\alpha \beta)^J f_J(\mathbf{r}, \mathbf{r}'), \quad \alpha, \beta = \text{const}. \quad (4)$$

One can prove that f_J satisfies the Laplace equation with respect to both vectors \mathbf{r} and \mathbf{r}' . Indeed,

$$\Delta' f_J = J r^{2J+d-2} (\nabla \cdot \nabla') (\mathbf{r}' \cdot \nabla)^{J-1} \frac{1}{r^{d-2}} = J(J-1) r^{2J+d-2} \Delta (\mathbf{r}' \cdot \nabla)^{J-2} \frac{1}{r^{d-2}} = 0. \quad (5)$$

Here, Δ' and ∇' act on the components of \mathbf{r}' . We have also used the identity $\Delta r^{2-d} = 0$ and the fact that the differential operations are commutative. The proof of $\Delta f_J = 0$ is somewhat more lengthy,

$$\Delta f_J = 2(2J+d-2) \left(\frac{(J+d-2)}{r^2} f_J + r^{2J+d-3} (\mathbf{r} \cdot \nabla) (\mathbf{r}' \cdot \nabla)^J \frac{1}{r^{d-2}} \right). \quad (6)$$

Using the operator identity

$$(\mathbf{r}' \cdot \nabla)^J (\mathbf{r} \cdot \nabla) = J (\mathbf{r}' \cdot \nabla)^J + (\mathbf{r} \cdot \nabla) (\mathbf{r}' \cdot \nabla)^J \quad (7)$$

one can transform the second term in (6) to

$$(\mathbf{r} \cdot \nabla) (\mathbf{r}' \cdot \nabla)^J \frac{1}{r^{d-2}} = [(\mathbf{r}' \cdot \nabla)^J (\mathbf{r} \cdot \nabla) - J (\mathbf{r}' \cdot \nabla)^J] \frac{1}{r^{d-2}} = -(J+d-2) (\mathbf{r}' \cdot \nabla)^J \frac{1}{r^{d-2}}. \quad (8)$$

The substitution of this identity into (6) completes the proof of the equation $\Delta f_J = 0$.

The scalar function $f_J(\mathbf{r}, \mathbf{r}')$ is J th order homogeneous polynomial satisfying the Laplace equations $\Delta f_J = \Delta' f_J = 0$, therefore, it can be nothing else than the scalar product of two HSHs of rank J ,

$$f_J(\mathbf{r}, \mathbf{r}') = (r r')^J \sum_{\epsilon} [H_{\epsilon}^J(\hat{\mathbf{r}}')]^* H_{\epsilon}^J(\hat{\mathbf{r}}). \quad (9)$$

The explicit form of f_J can be calculated as follows. First, we note that the gradient operators in (3) can be replaced with the derivatives,

$$f_J = r^{2J+d-2} \frac{d^J}{dt^J} \frac{1}{|\mathbf{r} + t \mathbf{r}'|^{d-2}} \Big|_{t=0} = \frac{d^J}{dt^J} \frac{(-1)^J r^{2J}}{(1 - 2\xi(tr'/r) + (tr'/r)^2)^{d/2-1}} \Big|_{t=0}, \quad (10)$$

where $\xi = (\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}})$ is the cosine of the angle between \mathbf{r}' and \mathbf{r} . Noting that the function to be differentiated coincides with the generating function for Gegenbauer (or ultraspherical) polynomials⁶ we can write

$$f_J = (-1)^J r^{2J} \frac{d^J}{dt^J} \sum_{n=0}^{\infty} \left(\frac{tr'}{r} \right)^n C_n^{d/2-1}(\xi) \Big|_{t=0} = (-r r')^J J! C_J^{d/2-1}(\xi). \quad (11)$$

At this stage, we note that HSHs are defined up to a normalization factor which can be an arbitrary number independent of r, r' . Thus, the scalar product of HSH (9) is expressed as

$$\sum_{\epsilon} [H_{\epsilon}^J(\hat{\mathbf{r}}')]^* H_{\epsilon}^J(\hat{\mathbf{r}}) = A_J^{(d)} C_J^{d/2-1}(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}}), \tag{12}$$

where $A_J^{(d)}$ is the normalization constant and $C_J^{d/2-1}(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}})$ is the J th order Gegenbauer polynomial.

B. The construction of d -dimensional HSH

The main idea is based on the fact that the scalar product $(\mathbf{a} \cdot \mathbf{r})^J$ for zero-length vectors \mathbf{a} [i.e., for $(\mathbf{a} \cdot \mathbf{a})=0$] satisfies the Laplace equation. The proof is very simple,

$$\Delta(\mathbf{a} \cdot \mathbf{r})^J = J(\mathbf{a} \cdot \nabla)(\mathbf{a} \cdot \mathbf{r})^{J-1} = J(J-1)(\mathbf{a} \cdot \mathbf{a})(\mathbf{a} \cdot \mathbf{r})^{J-2} = 0. \tag{13}$$

The condition $(\mathbf{a} \cdot \mathbf{a})=0$ means that some components of the zero-length vector \mathbf{a} must be complex numbers. Let us choose the components of \mathbf{a} to be

$$\mathbf{a} = (\hat{\mathbf{b}}_{\kappa}, i\hat{\mathbf{b}}_{d-\kappa}), \quad \kappa < d, \tag{14}$$

where d is the dimensionality of \mathbf{a} and \mathbf{r} . The *real* unit vectors $\hat{\mathbf{b}}_{\kappa}$ and $\hat{\mathbf{b}}_{d-\kappa}$ have dimensionalities κ and $d-\kappa$, respectively. It is easy to see that the zero-length condition is met

$$\mathbf{a} \cdot \mathbf{a} = (\hat{\mathbf{b}}_{\kappa})^2 + (i\hat{\mathbf{b}}_{d-\kappa})^2 = 1 - 1 = 0. \tag{15}$$

Let us parametrize the d -dimensional radius vector \mathbf{r} as

$$\mathbf{r} = (\mathbf{r}_{\kappa}, \mathbf{r}_{d-\kappa}). \tag{16}$$

It is more convenient to work with unit vectors so that

$$\mathbf{r}_{\kappa} = r_{\kappa} \hat{\mathbf{r}}_{\kappa} = r \cos \theta_{\kappa} \hat{\mathbf{r}}_{\kappa},$$

$$\mathbf{r}_{d-\kappa} = r_{d-\kappa} \hat{\mathbf{r}}_{d-\kappa} = r \sin \theta_{\kappa} \hat{\mathbf{r}}_{d-\kappa}, \tag{17}$$

where $\theta_{\kappa} \in [0, \pi/2]$ and the hyper-radius is defined by $r^2 = r_{\kappa}^2 + r_{d-\kappa}^2 = \sum_{n=1}^d x_n^2$. Note that the above parametrization implies that $\kappa > 1$ and $(d-\kappa) > 1$. It is important to note that we are not making any assumptions about the parametrization of the unit vectors $\hat{\mathbf{r}}_{\kappa}$ and $\hat{\mathbf{r}}_{d-\kappa}$.

Suppose that explicit expressions for HSH with the dimensionalities κ , $(d-\kappa)$ are known. Then, one can obtain an expression for the d -dimensional HSH as the product of known HSH with some weight function. We begin the proof of this statement by writing

$$(\mathbf{a} \cdot \mathbf{r})^J = [(\hat{\mathbf{b}}_{\kappa} \cdot \mathbf{r}_{\kappa}) + i(\hat{\mathbf{b}}_{d-\kappa} \cdot \mathbf{r}_{d-\kappa})]^J = \sum_{q=0}^J \binom{J}{q} i^{J-q} (\hat{\mathbf{b}}_{\kappa} \cdot \mathbf{r}_{\kappa})^q (\hat{\mathbf{b}}_{d-\kappa} \cdot \mathbf{r}_{d-\kappa})^{J-q}. \tag{18}$$

Now we expand the scalar products over the Gegenbauer polynomials which, in turn, are the scalar products of HSH. Namely,

$$(\hat{\mathbf{b}}_{\kappa} \cdot \mathbf{r}_{\kappa})^q = r_{\kappa}^q \sum_{l=0}^q B_{ql}^{(\kappa)} C_l^{\kappa/2-1}(\hat{\mathbf{b}}_{\kappa} \cdot \hat{\mathbf{r}}_{\kappa}) = r_{\kappa}^q \sum_{l=0}^q \frac{B_{ql}^{(\kappa)}}{A_l^{(\kappa)}} \sum_{\epsilon} [H_{\epsilon}^l(\hat{\mathbf{b}}_{\kappa})]^* H_{\epsilon}^l(\hat{\mathbf{r}}_{\kappa}). \tag{19}$$

Here, ϵ denotes the set of $(\kappa-2)$ projection indices of HSH, $B_{ql}^{(\kappa)}$ are the expansion coefficients which can be calculated using the orthogonality of Gegenbauer polynomials. Omitting details of the computations, we present only the final expression for $B_{ql}^{(\kappa)}$,

$$B_{ql}^{(\kappa)} = \sigma_{q,l} \frac{q! (l + \kappa/2 - 1) \Gamma(\kappa/2 - 1) \Gamma(n + 1/2)}{\sqrt{\pi} 2^l (q-l)! \Gamma(l + \kappa/2 + n)}, \quad q-l = 2n, \tag{20}$$

where integer $n \geq 0$ and $\sigma_{q,l} = [1 + (-1)^{q-l}]/2$. Thus, $B_{ql}^{(\kappa)} = 0$ if q and l have different parities.

Substituting Eq. (19) and the similar equation for $(\hat{\mathbf{b}}_{d-\kappa} \cdot \mathbf{r}_{d-\kappa})^{J-q}$ into (18), the scalar product $(\mathbf{a} \cdot \mathbf{r})^J$ can be written as

$$(\mathbf{a} \cdot \mathbf{r})^J = r^J \sum_{l,l'} [H_\epsilon^l(\hat{\mathbf{b}}_\kappa) H_{\epsilon'}^{l'}(\hat{\mathbf{b}}_{d-\kappa})]^* \frac{H_{l\epsilon,l'\epsilon'}^J(\hat{\mathbf{r}})}{A_l^{(\kappa)} A_{l'}^{(d-\kappa)}}, \quad (21)$$

where the functions $H_{l\epsilon,l'\epsilon'}^J(\hat{\mathbf{r}})$ are defined by the product

$$H_{l\epsilon,l'\epsilon'}^J(\hat{\mathbf{r}}) = H_\epsilon^l(\hat{\mathbf{r}}_\kappa) H_{\epsilon'}^{l'}(\hat{\mathbf{r}}_{d-\kappa}) h_{ll'}^J(\theta_\kappa), \quad (22)$$

where $h_{ll'}^J(\theta_\kappa)$ denotes the summation

$$h_{ll'}^J(\theta_\kappa) = \sum_q \binom{J}{q} i^{J-q} (\cos \theta_\kappa)^q (\sin \theta_\kappa)^{J-q} B_{ql}^{(\kappa)} B_{(J-q)l'}^{(d-\kappa)}. \quad (23)$$

Noting that the action of the Laplace operator on (21) gives $\Delta(\mathbf{a} \cdot \mathbf{r})^J = 0$, and, since $\hat{\mathbf{b}}_\kappa$ and $\hat{\mathbf{b}}_{d-\kappa}$ are arbitrary vectors, we arrive at the identity

$$\Delta[r^J H_{l\epsilon,l'\epsilon'}^J(\hat{\mathbf{r}})] = 0. \quad (24)$$

Therefore, $H_{l\epsilon,l'\epsilon'}^J$ are d -dimensional HSH of the rank J with projection indices $l\epsilon, l'\epsilon'$.

The explicit form of the functions $h_{ll'}^J(\theta_\kappa)$ defined by (23) is derived in the Appendix A, where it is shown that $h_{ll'}^J$ are proportional to the Jacobi polynomials; see Eq. (A2).

The above consideration was performed under an assumption that $\kappa > 1$ and $d - \kappa > 1$. Thus, the case $\kappa = 1$ needs special consideration. First, we parametrize the radius vector \mathbf{r} as

$$\mathbf{r} = r(\cos \theta, \sin \theta \hat{\mathbf{r}}_{d-1}), \quad \theta \in [0, \pi]. \quad (25)$$

Again, no assumptions are made about the parametrization of the components of the unit $(d-1)$ -dimensional vector $\hat{\mathbf{r}}_{d-1}$.

We choose the parametrization of the zero-length vector \mathbf{a} to be

$$\mathbf{a} = (1, i\hat{\mathbf{b}}), \quad (26)$$

where $\hat{\mathbf{b}}$ is the unit real $(d-1)$ -dimensional vector. The expansion of the scalar product $(\mathbf{a} \cdot \mathbf{r})^J$ has the form

$$(\mathbf{a} \cdot \mathbf{r})^J = r^J [1 + i(\hat{\mathbf{b}} \cdot \mathbf{r}_{d-1})]^J = \sum_{q=0}^J \binom{J}{q} i^{J-q} (\cos \theta)^{J-q} (\sin \theta)^{J-q} (\hat{\mathbf{b}} \cdot \mathbf{r}_{d-1})^q. \quad (27)$$

Decomposing the scalar product $(\hat{\mathbf{b}} \cdot \mathbf{r}_{d-1})^q$ using Eq. (19) (where $\kappa = d-1$), we can rewrite the above equation as

$$(\mathbf{a} \cdot \mathbf{r})^J = r^J \sum_l [H_\epsilon^l(\hat{\mathbf{b}})]^* \frac{H_{l\epsilon}^J(\hat{\mathbf{r}})}{A_l^{(d-\kappa)}}, \quad (28)$$

where the d -dimensional HSH $H_{l\epsilon}^J(\hat{\mathbf{r}})$ is the product of $(d-1)$ -dimensional HSH and the function of θ ,

$$H_{l\epsilon}^J(\hat{\mathbf{r}}) = g_l^J(\theta) H_\epsilon^l(\hat{\mathbf{r}}_{d-1}), \quad (29)$$

where $g_l^J(\theta)$ are defined similarly to (23),

$$g_l^J(\theta) = \sum_q \binom{J}{q} i^{J-q} (\cos \theta)^q (\sin \theta)^{J-q} B_{ql}^{(d-1)}. \quad (30)$$

This summation evaluates in a closed form as the Gegenbauer polynomial; see Eq. (A5) of Appendix A.

C. Orthogonality and normalization

It is important that HSH defined by (22) form an orthogonal set on the d -dimensional hypersphere. In order to demonstrate this, we have to derive the expression for the surface element on the hypersphere, as follows:

$$d\mathbf{r} = r^{d-1} dr d\Omega_d = d\mathbf{r}_\kappa d\mathbf{r}_{d-\kappa} = r_\kappa^{\kappa-1} dr_\kappa r_{d-\kappa}^{d-\kappa-1} dr_{d-\kappa} d\Omega_\kappa d\Omega_{d-\kappa}. \quad (31)$$

Noting that $dr_\kappa dr_{d-\kappa} = r dr d\theta_\kappa$ and using the hyperspherical parametrization (17) of $r_\kappa, r_{d-\kappa}$, we find the surface element of the d -dimensional hypersphere to be

$$d\Omega_d = (\cos \theta_\kappa)^{\kappa-1} (\sin \theta_\kappa)^{d-\kappa-1} d\theta_\kappa d\Omega_\kappa d\Omega_{d-\kappa}. \quad (32)$$

The orthogonality of HSH (22) follows from the orthogonality of κ - and $(d-\kappa)$ -dimensional HSH and properties of Jacobi polynomials.⁶ The same is also true for HSH defined by (29).

Assuming that κ - and $(d-\kappa)$ -dimensional HSH $H_\epsilon^l(\hat{\mathbf{r}}_\kappa)$ and $H_{\epsilon'}^{l'}(\hat{\mathbf{r}}_{d-\kappa})$ are normalized, the normalized d -dimensional HSH can be written as

$$Y_{l\epsilon, l'\epsilon'}^J(\hat{\mathbf{r}}) = H_\epsilon^l(\hat{\mathbf{r}}_\kappa) H_{\epsilon'}^{l'}(\hat{\mathbf{r}}_{d-\kappa}) y_{ll'}^J(\theta_\kappa), \quad (33)$$

where the functions $y_{ll'}^J$ are proportional to Jacobi polynomials $P_\lambda^{(\alpha, \beta)}$,

$$y_{ll'}^J(\theta_\kappa) = N_{ll'}^{(d, \kappa)} (\cos \theta_\kappa)^l (\sin \theta_\kappa)^{l'} P_\lambda^{(l'-1+d-\kappa/2, l-1+\kappa/2)}(\cos 2\theta_\kappa), \quad (34)$$

where $\lambda = (J-l-l')/2$. Note that $y_{ll'}^J$ is nonzero only when λ is an integer number. The normalization constant in the above equation is defined by

$$N_{ll'}^{(d, \kappa)} = \left[\frac{(2J-2+d)\lambda! \Gamma(\lambda+l+l'+d/2-1)}{\Gamma(\lambda+l'+(d-\kappa)/2) \Gamma(\lambda+l+\kappa/2)} \right]^{1/2}. \quad (35)$$

The orthogonality relation for functions $y_{ll'}^J(\theta_\kappa)$ has the form

$$\int_0^{\pi/2} y_{ll'}^J(\theta_\kappa) y_{l'l}^J(\theta_\kappa) (\cos \theta_\kappa)^{\kappa-1} (\sin \theta_\kappa)^{d-\kappa-1} d\theta_\kappa = \delta_{J, l'l}. \quad (36)$$

In the case $\kappa=1$ the orthonormal HSH can be written as the product of $(d-1)$ -dimensional normalized HSH $H_\epsilon^l(\hat{\mathbf{r}}_{d-1})$ and the function $y_l^J(\theta)$,

$$Y_{l\epsilon}^J(\hat{\mathbf{r}}) = y_l^J(\theta) H_\epsilon^l(\hat{\mathbf{r}}_{d-1}),$$

$$y_l^J(\theta) = N_{ll}^{(d)} (\sin \theta)^l C_{J-l}^{l+d-1/2}(\cos \theta), \quad (37)$$

where $C_{J-l}^{l+d-1/2}(\cos \theta)$ is the Gegenbauer polynomial and the normalization coefficient is given by

$$N_{ll}^{(d)} = \Gamma\left(l + \frac{d-1}{2}\right) \left[\frac{2^{2l+d} (J+(d-1)/2)(J-l)!}{4\pi (J+l+d-2)!} \right]^{1/2}. \quad (38)$$

The orthogonality relation for the functions y_l^J reads

$$\int_0^\pi y_l^J(\theta) y_l^{J'}(\theta) (\sin \theta)^{d-1} d\theta = \delta_{J,J'}. \quad (39)$$

The above Eqs. (33)–(39) constitute the main results of the presented paper.

III. HSH IN SPACES WITH $d=2, \dots, 6$

Below we consider HSH in spaces with dimensionalities from two to six. This is necessary in order to establish the connection of the derived HSH with the expressions existing in literature (if any).

A. Two- and three-dimensional HSHs

The zero-length vector $\mathbf{a}=(1, i)$ and the radius vector $\mathbf{r}=(x, y)$. Their scalar product is

$$(\mathbf{a} \cdot \mathbf{r})^m = (x + iy)^m = r^m e^{im\phi}, \quad (40)$$

where ϕ is the polar angle, $\phi \in [0, 2\pi)$. Thus, the two-dimensional (2D) spherical (or better, circular) normalized harmonics are

$$Y_m(\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}. \quad (41)$$

Note that $m \geq 0$ is the rank of HSH. However, by considering $\mathbf{a}=(1, -i)$ one obtains that $\exp(-m\phi)$ is HSH, too. Therefore, in (41) the index m can be $\pm 1, \pm 2, \dots$. Note also that $Y_m(-\phi) = Y_{-m}(\phi) = Y_m^*(\phi)$.

The above expression for the 2D HSH allows one to obtain 3D HSH by using Eq. (37) of Sec. II C. The radius vector \mathbf{r} we decompose into the direct product of the one component parameter $\cos \theta$ and 2D vector, so that

$$\mathbf{r} = r(\cos \theta, \sin \theta \hat{\mathbf{r}}_2) = r(\cos \theta, \sin \theta \cos \phi, \sin \theta \sin \phi). \quad (42)$$

Inserting $d=2$ and $l=m$ into Eqs. (37) and (38), we obtain

$$Y_m^J(\hat{\mathbf{r}}) = Y_m^J(\theta, \phi) = (2m-1)!! \sqrt{\frac{2J+1}{4\pi} \frac{(J-m)!}{(J+m)!}} e^{im\phi} (\sin \theta)^m C_{J-m}^{m+1/2}(\cos \theta). \quad (43)$$

These functions differ from the conventional spherical harmonics $Y_{Jm}(\theta, \phi)$ only by the phase factor $(-1)^m$. Clearly, all properties of Y_m^J are the same as those of spherical harmonics (see, e.g., Ref. 13) and we will not discuss them further.

B. Four-dimensional HSH

The importance of the four-dimensional (4D) HSH stems from the fact that they represent the wave function of the hydrogen atom in the momentum space.¹⁴ Also, in the momentum space, HSH can be used as the Sturmian basis set which was successfully applied to many problems of quantum physics and chemistry.^{1,5,15,16}

There are two possibilities of representing the 4D-vector: it can be split into either (1+3)- or (2+2)-dimensional vectors. Below, the explicit expressions for the corresponding HSH are derived.

1. The parametrization by 1D+3D vectors

The radius vector is $\mathbf{R}=(\cos \omega, \sin \omega \hat{\mathbf{r}})$, where $\hat{\mathbf{r}}=(\cos \theta, \sin \theta \cos \phi, \sin \theta \sin \phi)$ is the unit 3D vector. For such parametrization, according to Eqs. (37) and (38), we have

$$Y_{lm}^J(\hat{\mathbf{R}}) = Y_{lm}^J(\omega, \theta, \phi) = l! \sqrt{\frac{2(J+1)(J-l)!}{\pi(J+l+1)!}} (2 \sin \omega)^l C_{J-l}^{l+1}(\cos \omega) Y_{lm}(\theta, \phi). \quad (44)$$

The orthogonality relation for these harmonics has the form

$$\int_0^\pi (\sin \omega)^2 d\omega \int_0^\pi \sin \theta d\theta \int_0^{2\pi} d\phi [Y_{lm}^J(\omega, \theta, \phi)]^* Y_{l'm'}^J(\omega, \theta, \phi) = \delta_{J,J'} \delta_{l,l'} \delta_{m,m'}. \quad (45)$$

2. The parametrization by two 2D-vectors

In this section we derive the expression for 4D HSH depending on the angles of the radius vector \mathbf{R} represented by the two 2D vectors \mathbf{r}_1 and \mathbf{r}_2 ,

$$\mathbf{R} = (\mathbf{r}_1, \mathbf{r}_2), \quad \mathbf{r}_1 = r_1(\cos \phi_1, \sin \phi_1), \quad \mathbf{r}_2 = r_2(\cos \phi_2, \sin \phi_2), \quad (46)$$

where $\phi_1, \phi_2 \in [0, 2\pi)$. We parametrize the lengths $r_{1,2}$ by the hyper-radius $R = \sqrt{r_1^2 + r_2^2}$ and the hyperangle β as

$$r_1 = R \cos \beta, \quad r_2 = R \sin \beta, \quad \beta \in [0, \pi/2). \quad (47)$$

In these coordinates, the integration over the 4D hypersphere is given by (32) which in the above variables reads

$$\int d\Omega_4 = \frac{1}{2} \int_0^{\pi/2} \sin 2\beta d\beta \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2. \quad (48)$$

According to Eqs. (33)–(35) the orthonormal HSH take the form

$$Y_{m_1 m_2}^J(\hat{\mathbf{R}}) = Y_{m_1 m_2}^J(\beta, \phi_1, \phi_2) = \frac{1}{\pi} \left[\frac{(J+1)\lambda! (\lambda + m_1 + m_2)!}{2(\lambda + m_1)! (\lambda + m_2)!} \right]^{1/2} e^{i(m_1 \phi_1 + m_2 \phi_2)} \times (\cos \beta)^{m_1} (\sin \beta)^{m_2} P_\lambda^{(m_2, m_1)}(\cos 2\beta), \quad (49)$$

where $\lambda = (J - m_1 - m_2)/2$ must be an integer number; otherwise $Y_{m_1 m_2}^J = 0$. Note also that this definition is valid for $m_1, m_2 \geq 0$. For negative values of indices the replacement $\phi \rightarrow -\phi$ must be used, e.g.,

$$Y_{-m_1 m_2}^J(\beta, \phi_1, \phi_2) = Y_{m_1 m_2}^J(\beta, -\phi_1, \phi_2). \quad (50)$$

By comparing Eq. (49) with the definition of the Wigner d -function [Eq. (4.3.4.13) of Ref. 13], one sees that they coincide up to some constant factor. Thus, one can choose the 4D HSH to be

$$Y_{j\mu\nu}(\phi_1, \beta, \phi_2) = e^{i(\mu+\nu)\phi_1} d_{\mu\nu}^j(2\beta) e^{i(\mu-\nu)\phi_2}, \quad (51)$$

where j can be both integer and half-integer and the indices $\mu, \nu = -j, -j+1, \dots, j$. The connection of the quantum numbers $j\mu\nu$ with Jm_1m_2 has the form

$$j = \frac{J}{2}, \quad \mu = -\frac{m_1 + m_2}{2}, \quad \nu = \frac{m_2 - m_1}{2}. \quad (52)$$

HSH defined by (51) are orthogonal,

$$\int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \int_0^{\pi/2} (\sin \beta d\beta) [Y_{j\mu\nu}(\phi_1, \beta, \phi_2)]^* Y_{j'\mu'\nu'}(\phi_1, \beta, \phi_2) = \frac{8\pi^2}{2j+1} \delta_{jj'} \delta_{\mu,\mu'} \delta_{\nu,\nu'}. \quad (53)$$

The scalar product of HSH (51) has the form

$$(Y_j(\hat{\mathbf{R}}) \cdot Y_j(\hat{\mathbf{R}}')) = \sum_{\mu, \nu=-j}^j Y_{j\mu\nu}^*(\hat{\mathbf{R}}) Y_{j\mu\nu}(\hat{\mathbf{R}}') = \chi^j(\cos \omega), \quad (54)$$

where $\chi^j(\cos \omega)$ is the character of the $O(3)$ group¹³ and

$$\cos \omega = (\hat{\mathbf{R}} \cdot \hat{\mathbf{R}}') = \cos \beta \cos \beta' \cos(\phi_1 - \phi_1') + \sin \beta \sin \beta' \cos(\phi_2 - \phi_2'), \quad (55)$$

where ω is the angle between 4D vectors \mathbf{R} and \mathbf{R}' . For the sake of completeness we also present the explicit expression for the character,¹³ as follows:

$$\chi^j(\cos \omega) = C_{2j}^1(\cos \omega) = \frac{\sin[(2j+1)\omega]}{\sin \omega}. \quad (56)$$

We recall that the rank of HSH $Y_{j\mu\nu}$ defined by (51) is equal to $2j$.

Thus, we have proved that the 4D HSH parametrized by the pair of 2D vectors coincide with the Wigner D -functions which describe the transformation of the 3D harmonics under the rotation of the coordinate frame.¹³ This fact has many important consequences. For example, the Clebsch–Gordan coefficients for the 4D HSH can easily be obtained from the addition theorem for D -functions.¹⁷

C. Five-dimensional HSH

The five-dimensional (5D) space is of less importance from the point of view of physical applications. However, it can play a role in the quantum problem of two interacting particles, one of which is moving in the physical space and the other one being restricted to a surface.

Accordingly, it is convenient to parametrize 5D-vector \mathbf{R} as the direct product of 2D- and 3D-vectors,

$$\mathbf{R} = (\mathbf{r}_2, \mathbf{r}_3) = R(\cos \beta \hat{\mathbf{r}}_2, \sin \beta \hat{\mathbf{r}}_3), \quad (57)$$

where the unit vectors are

$$\hat{\mathbf{r}}_2 = (\cos \alpha, \sin \alpha), \quad \hat{\mathbf{r}}_3 = (\cos \theta, \sin \theta \cos \phi, \sin \theta \sin \phi). \quad (58)$$

The corresponding expression for 5D HSH can be obtained from Eqs. (33)–(35) upon the substitutions $d=5$ and $\kappa=2$,

$$Y_{\mu lm}^J(\hat{\mathbf{R}}) = \left[\frac{(2J+3)\lambda! (J+l+\mu+1)!!}{\pi 2^{\mu+1} (\lambda+\mu)! (J+l-\mu+1)!!} \right]^{1/2} e^{i\mu\alpha} (\cos \beta)^\mu (\sin \beta)^l P_\lambda^{(l+1/2, \mu)}(\cos 2\beta) \times Y_{lm}(\theta, \phi), \quad \lambda = \frac{J-l-\mu}{2}. \quad (59)$$

HSH $Y_{\mu lm}^J(\hat{\mathbf{R}})$ are nonzero only for integer values of λ . The above definition of HSH is valid for $\mu \geq 0$. In the opposite case the replacement $\alpha \rightarrow -\alpha$ must be done in (59) so that

$$Y_{-\mu lm}^J(\alpha, \beta, \theta, \phi) = Y_{\mu lm}^J(-\alpha, \beta, \theta, \phi). \quad (60)$$

D. Six-dimensional HSH

The dimensionality of the three-body problem after the separation of the c.m. motion is equal to six. Furthermore, the dimensionality of the kinetic-energy operator in the four-body problem can also be reduced to six after the separation of the collective rotations and c.m. motion. This explains the importance of 6D HSH.

Thus, the natural choice of the arguments of HSH would be the pair of 3D spherical angles plus the hyperangle describing the ratio of 3D vectors (Sec. III D 1).

However, if the planar systems are considered, most useful would be the parametrization in terms of three planar angles plus two hyperangles (Sec. III D 2).

1. The parametrization by two three-dimensional vectors

The 6D radius vector is $\mathbf{R}=R(\cos \alpha \hat{\mathbf{r}}_1, \sin \alpha \hat{\mathbf{r}}_2)$, where $\hat{\mathbf{r}}_{1,2}$ are unit 3D vectors which can be, e.g., Jacobi vectors of three particles; see Fig. 1.

The integration over the solid angle of the 6D hypersphere in these coordinates has the form

$$\int d\Omega_6 = \frac{1}{4} \int_0^{\pi/2} (\sin 2\alpha)^2 d\alpha \prod_{k=1}^2 \int_0^\pi \sin \theta_k d\theta_k \int_0^{2\pi} d\phi_k, \quad (61)$$

where $\theta_k \phi_k$ are the spherical angles of the unit vector $\hat{\mathbf{r}}_k$, $k=1, 2$.

The expression for the orthonormal HSH is given by Eqs. (33)–(35) where $d=6$, $\kappa=3$, so that

$$Y_{l_1 m_1 l_2 m_2}^J(\alpha, \hat{\mathbf{r}}_1, \hat{\mathbf{r}}_2) = \left[\frac{2^{J+3} (J+2) \lambda! (\lambda + l_1 + l_2 + 1)!}{\pi (J + l_1 - l_2 + 1)! (J - l_1 + l_2 + 1)!} \right]^{1/2} \\ \times (\cos \alpha)^{l_1} (\sin \alpha)^{l_2} P_\lambda^{(l_2+1/2, l_1+1/2)}(\cos 2\alpha) Y_{l_1 m_1}(\hat{\mathbf{r}}_1) Y_{l_2 m_2}(\hat{\mathbf{r}}_2). \quad (62)$$

Note that HSH are nonzero only for integer values of $\lambda=(J-l_1-l_2)/2 \geq 0$.

2. The parametrization by three two-dimensional vectors

We parametrize the radius vector as $\mathbf{R}=(\mathbf{r}_1, \mathbf{R}_4)$, where $\mathbf{r}_1=r_1(\cos \phi_1, \sin \phi_1)$ and \mathbf{R}_4 is 4D-vector composed of two 2D-vectors so that

$$\mathbf{R}_4 = (\mathbf{r}_2, \mathbf{r}_3) = (r_2 \cos \phi_2, r_2 \sin \phi_2, r_3 \cos \phi_3, r_3 \sin \phi_3). \quad (63)$$

It is necessary to specify the parametrization of the lengths r_1, r_2, r_3 . We choose it to be

$$r_1 = R \cos \theta, \quad r_2 = R \sin \theta \cos \beta, \quad r_3 = R \sin \theta \sin \beta, \quad (64)$$

where $\theta, \beta \in [0, \pi/2)$ and $R^2=r_1^2+r_2^2+r_3^2$. The integration over the angles of the 6D hypersphere in the above coordinates has the form

$$\int d\Omega_6 = \frac{1}{4} \int_0^{\pi/2} (\sin \theta)^2 \sin 2\theta d\theta \int_0^{\pi/2} \sin 2\beta d\beta \prod_{k=1}^3 \int_0^{2\pi} d\phi_k. \quad (65)$$

Using Eqs. (33)–(35), where $d=6$, $\kappa=2$, the orthonormal HSH can be written as

$$Y_{l, m_1 m_2 m_3}^J(\theta, \beta, \phi_1, \phi_2, \phi_3) = \left[\frac{(J+2) \lambda! (\lambda + m_1 + l + 1)!}{\pi (\lambda + m_1)! (\lambda + l + 1)!} \right]^{1/2} e^{im_1 \phi_1} (\cos \theta)^{m_1} (\sin \theta)^l \\ \times P_\lambda^{(l+1, m_1)}(\cos 2\theta) Y_{m_2 m_3}^l(\beta, \phi_2, \phi_3). \quad (66)$$

These functions are nonzero at non-negative integer values of $\lambda=(J-m_1-l)/2$ and $(l-m_2-m_3)/2$. As a consequence, we have that $(J-m_1-m_2-m_3)/2$ must also be a non-negative integer number. In (66) the 4D HSH $Y_{m_2 m_3}^l(\beta, \phi_2, \phi_3)$ can be defined by Eq. (49) of Sec. II. Again, the above Eq. (66) is valid only for $m_1 \geq 0$. In the opposite case one has

$$Y_{l,-m_1 m_2 m_3}^J(\theta, \beta, \phi_1, \phi_2, \phi_3) = Y_{l, m_1 m_2 m_3}^J(\theta, \beta, -\phi_1, \phi_2, \phi_3). \quad (67)$$

IV. CONCLUSION

In the presented paper the technique of the derivation of the HSH with arbitrary arguments has been developed. This technique does not require the tedious procedure of the transformation of the Laplace operator to the set of desired variables. It allows one to obtain the explicit expressions for HSH depending on the variables which are most suited to the problem under consideration. For example, in the helium atom problem the convenient set of variables comprises the spherical angles and lengths of the position vectors of the two electrons. In the calculation of the wave functions of three- and four-electron quantum dots the set of polar angles plus lengths of position vectors of electrons is convenient. In both problems above, HSH may serve as a basis for the expansion of the wave function in order to transform Schrödinger equation to the matrix form.

The main results of the paper are Eqs. (33)–(35), (37), and (38) of Sec. II which define orthogonal and normalized HSH in d -dimensional space in terms of products of lower-dimensional HSH. As examples of the derived representations, the explicit expressions for HSH in spaces with dimensions from two to six have been derived in Sec. III.

Expressions for the 4D HSH were presented for the two most important sets of variables; see Secs. III B 1 and III B 2. The importance of 4D HSH stems from the fact that they represent the wave functions of the hydrogen atom in momentum space.¹⁴

6D HSH depending on the spherical angles of two 3D vectors and the hyperangle describing their ratio are analyzed in Sec. III D 1. These HSHs are relevant to the quantum three-body problem.^{18,19} Note that 6D HSH given by the expression (62) are not eigenfunctions of the operator of total angular momentum $\mathbf{L} = -i([\mathbf{r}_1 \times \nabla_1] + [\mathbf{r}_2 \times \nabla_2])$. The set of HSH being eigenfunctions of \mathbf{L} can be constructed by taking the linear combination of HSH (62) with the conventional Clebsch–Gordan coefficients.¹³

The expression for the 6D HSH which can be useful in planar quantum three- and four-body problems is derived in Sec. III D 2. In this case, HSH depend on the polar angles of three coplanar vectors and the two hyperangles which describe the relative lengths of those vectors.

The application of HSH to N -body problems requires knowledge of the transformation properties of HSH under particle exchange. Such properties depend on the connection of the position vectors of particles with the hyperangles and in every particular situation must be analyzed separately. The procedure of the transformation of HSH under the particle exchange is often referred to as “kinematic rotation” and is discussed, e.g., in Refs. 8 and 20.

We emphasize that the method of zero-length vectors presented in Sec. II B is quite general and can be used in order to derive expressions for *arbitrary* sets of HSH, including nonorthogonal ones. Once the Cartesian components of the radius vector \mathbf{r} are parametrized in terms of the hyper-radius and hyperangles, J th rank HSH will be given by the coefficients in the expansion of the function $(\mathbf{r} \cdot \mathbf{a})^J$, where \mathbf{a} is an arbitrary constant zero-length vector, $(\mathbf{a} \cdot \mathbf{a}) = 0$. Probably, this gives the simplest approach to the calculation of HSH.

Finally, we note that the method proposed in this paper can also be applied to the problem of the calculation of Clebsch–Gordan coefficients in many-dimensional space. These coefficients allow one to evaluate many-dimensional integrals involving the products of HSH. Clebsch–Gordan coefficients are also necessary for the derivation of the multipole expansions of functions depending on several vector arguments. Examples of such multipole expansions of functions depending on $|\mathbf{R} - \mathbf{R}'|$ in 3D and 4D space may be found in Refs. 17 and 21.

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APPENDIX A: THE EXPLICIT FORM OF $h_{ll'}^J$ AND g_l^J

In this section we calculate the functions $h_{ll'}^J(\theta_\kappa)$ defined by Eq. (23) of the main text.

From the properties of the B -coefficients (20) it follows that $h_{ll'}^J(\theta_\kappa)=0$ for the combination $(J-l-l')=2\lambda$ being an *odd* number. Thus, λ must always be an integer.

Substituting Eq. (20) and the similar identity for $B_{(J-q)l'}^{(d-\kappa)}$ into Eq. (23), after some simple transformations, we obtain

$$h_{ll'}^J(\theta_\kappa) = i^{l'} 2^{-J} \sum_{n=0}^{\lambda} (-1)^{\lambda+n} \frac{(l+\kappa/2-1)\Gamma(\kappa/2-1)}{n!(\lambda-n)!\Gamma(n+l+\kappa/2)} \frac{(l'+(d-\kappa)/2-1)\Gamma((d-\kappa)/2-1)}{\Gamma(\lambda-n+l'+(d-\kappa)/2)} \times (\cos \theta_\kappa)^{l+2n} (\sin \theta_\kappa)^{l'+2\lambda-2n}. \quad (\text{A1})$$

Here, the summation leads to the Jacobi polynomial,⁶

$$h_{ll'}^J(\theta_\kappa) = A_{\lambda ll'}^{(d,\kappa)} (\cos \theta_\kappa)^l (\sin \theta_\kappa)^{l'} P_{\lambda}^{(l'-1+[(d-\kappa)/2], l-1+(\kappa/2))}(\cos 2\theta_\kappa), \quad (\text{A2})$$

where the coefficient $A_{\lambda ll'}^{(d,\kappa)}$ is

$$A_{\lambda ll'}^{(d,\kappa)} = \frac{i^{l'} (l+\kappa/2-1)(l'+(d-\kappa)/2-1)\Gamma(\kappa/2-1)\Gamma((d-\kappa)/2-1)}{2^J \Gamma(\lambda+l'+(d-\kappa)/2)\Gamma(\lambda+l+\kappa/2)}. \quad (\text{A3})$$

The explicit expression for the function g_l^J defined in (30) is

$$g_l^J(\theta) = i^{l'} 2^{-J} J! \left(l + \frac{d-3}{2} \right) \Gamma\left(\frac{d-3}{2} \right) \sum_{n=0} \frac{(-1)^n (\sin \theta)^{l+2n} (2 \cos \theta)^{J-l-2n}}{n! (J-l-2n)! \Gamma(l+n+d/2)}. \quad (\text{A4})$$

The sum over n evaluates to the Gauss hypergeometric function which is equivalent to the Gegenbauer polynomial,⁶

$$g_l^J(\theta) = A_{ll}^{(d)} (\sin \theta)^l C_{J-l}^{l+[(d-1)/2]}(\cos \theta), \quad (\text{A5})$$

where

$$A_{ll}^{(d)} = i^{l'} 2^{d+l-J-2} J! \left(l + \frac{d-3}{2} \right) \Gamma\left(\frac{d-3}{2} \right) \frac{\Gamma(l+(d-1)/2)}{\Gamma(J+l+d-1)}. \quad (\text{A6})$$

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