

Some integral identities for spherical harmonics in an arbitrary dimension

Weimin Han · Kendall Atkinson · Hao Zheng

Received: 15 July 2011 / Accepted: 9 December 2011 / Published online: 22 December 2011
© Springer Science+Business Media, LLC 2011

Abstract Spherical harmonics in an arbitrary dimension are employed widely in quantum theory. Spherical harmonics are also called hyperspherical harmonics when the dimension is larger than 3. In this paper, we derive some integral identities involving spherical harmonics in an arbitrary dimension.

Keywords Spherical harmonics · Funk-Hecke formula · Integral identity

1 Introduction

Spherical harmonics in an arbitrary dimension d , also called hyperspherical harmonics when the dimension $d \geq 4$, are employed widely in quantum theory, see e.g., [1, 3, 5, 7, 8, 11, 12], and also comprehensive presentations [4, 6]. The purpose of this paper is to present some integral identities involving spherical harmonics in an arbitrary dimension.

W. Han

Department of Mathematics and Program in Applied Mathematical and Computational Sciences,
University of Iowa, Iowa City, IA 52242, USA
e-mail: weimin-han@uiowa.edu

K. Atkinson

Department of Computer Science and Department of Mathematics, University of Iowa, Iowa City,
IA 52242, USA
e-mail: Kendall-Atkinson@uiowa.edu

H. Zheng (✉)

Department of Chemistry, Zhejiang University, Hangzhou 310027, China
e-mail: zhenghao@zju.edu.cn

First, we introduce some notation. The set

$$\mathbb{R}^d := \left\{ \mathbf{x} = (x_1, \dots, x_d)^d : x_j \in \mathbb{R}, 1 \leq j \leq d \right\}$$

is the d -dimensional Euclidean space, and

$$\mathbb{S}^{d-1} := \left\{ \boldsymbol{\xi} \in \mathbb{R}^d : |\boldsymbol{\xi}| = 1 \right\}$$

is the unit sphere in \mathbb{R}^d . Here $\boldsymbol{\xi} = (\xi_1, \dots, \xi_d)^T$ and

$$|\boldsymbol{\xi}| = \left(\sum_{i=1}^d |\xi_i|^2 \right)^{1/2}$$

is the Euclidean norm of $\boldsymbol{\xi}$. Generic points in \mathbb{S}^{d-1} will be denoted by $\boldsymbol{\xi}, \boldsymbol{\eta}$. We use the symbol \mathbb{Y}_n^d for the spherical harmonic space of order n in d dimensions. Any function in \mathbb{Y}_n^d is called a spherical harmonic of order n in d dimensions, and is the restriction to the unit sphere \mathbb{S}^{d-1} of a harmonic, homogeneous polynomial of degree n in the variable $\mathbf{x} \in \mathbb{R}^d$. Introduce a weighted norm

$$\|f\|_{L^1_{(d-3)/2}(-1,1)} := \int_{-1}^1 |f(t)|(1-t^2)^{(d-3)/2} dt$$

for a measurable function f on $(-1, 1)$, and then define $L^1_{(d-3)/2}(-1, 1)$ to be the weighted L^1 space of all measurable functions for which the norm $\|\cdot\|_{L^1_{(d-3)/2}(-1,1)}$ is finite. Note that for $d \geq 2$, any continuous function on $[-1, 1]$ belongs to the space $L^1_{(d-3)/2}(-1, 1)$. Throughout the paper, we assume the dimension $d \geq 2$.

Now we recall the Funk-Hecke formula which is useful in simplifying calculations of certain integrals over \mathbb{S}^{d-1} . A proof of this formula can be found in [10].

Theorem 1 (Funk-Hecke Formula) *Let $f \in L^1_{(d-3)/2}(-1, 1)$, $\boldsymbol{\xi} \in \mathbb{S}^{d-1}$ and $Y_n \in \mathbb{Y}_n^d$. Then the Funk-Hecke formula holds:*

$$\int_{\mathbb{S}^{d-1}} f(\boldsymbol{\xi} \cdot \boldsymbol{\eta}) Y_n(\boldsymbol{\eta}) dS^{d-1}(\boldsymbol{\eta}) = \lambda_n Y_n(\boldsymbol{\xi}) \tag{1}$$

with the constant λ_n given by

$$\lambda_n = |\mathbb{S}^{d-2}| \int_{-1}^1 P_{n,d}(t) f(t) (1-t^2)^{\frac{d-3}{2}} dt. \tag{2}$$

In (2), $|\mathbb{S}^{d-2}|$ denotes the surface area of the unit sphere in \mathbb{R}^{d-1} :

$$|\mathbb{S}^{d-2}| = \frac{2 \pi^{\frac{d-1}{2}}}{\Gamma\left(\frac{d-1}{2}\right)},$$

where $\Gamma(\cdot)$ is the Gamma function. Moreover,

$$P_{n,d}(t) = n! \Gamma\left(\frac{d-1}{2}\right) \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \frac{(1-t^2)^k t^{n-2k}}{4^k k! (n-2k)! \Gamma\left(k + \frac{d-1}{2}\right)}$$

is the Legendre polynomial of degree n in d dimensions. For a fixed dimension d , the Legendre polynomials $\{P_{n,d}\}_{n \geq 0}$ form an orthogonal basis in the weighted space $L^2_{(d-3)/2}(-1, 1)$ with the inner product

$$(f, g)_{L^2_{(d-3)/2}(-1,1)} := \int_{-1}^1 f(t) g(t) (1-t^2)^{(d-3)/2} dt.$$

For $d = 3$, $P_{n,3}(t)$ is the ordinary Legendre polynomial of degree n .

The Funk-Hecke formula is valid as long as the integral for λ_n exists, and this is certainly the case if $f \in \mathbb{C}[-1, 1]$.

To apply the Funk-Hecke formula, we need the Rodrigues representation formula for the Legendre polynomial

$$P_{n,d}(t) = (-1)^n R_{n,d} (1-t^2)^{\frac{3-d}{2}} \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\frac{d-3}{2}} \quad \text{for } d \geq 2, \tag{3}$$

where the Rodrigues constant

$$R_{n,d} = \frac{\Gamma\left(\frac{d-1}{2}\right)}{2^n \Gamma\left(n + \frac{d-1}{2}\right)}. \tag{4}$$

2 A family of integral identities for spherical harmonics

Throughout the paper, we denote by $Y_n \in \mathbb{Y}_n^d$ an arbitrary spherical harmonic of order n in d dimensions. Consider an integral of the form

$$I(g)(\xi) := \int_{\mathbb{S}^{d-1}} g(|\xi - \eta|) Y_n(\eta) dS^{d-1}(\eta). \tag{5}$$

We have the following result.

Proposition 2 *Assume*

$$g(2^{1/2}(1-t)^{1/2}) \in L^1_{(d-3)/2}(-1, 1). \tag{6}$$

Then

$$I(g)(\xi) = \mu_n Y_n(\xi), \tag{7}$$

where

$$\mu_n = |\mathbb{S}^{d-2}| \int_{-1}^1 g(2^{1/2}(1-t)^{1/2}) P_{n,d}(t) (1-t^2)^{\frac{d-3}{2}} dt. \tag{8}$$

Proof Since

$$|\xi - \eta| = [2(1 - \xi \cdot \eta)]^{1/2}, \quad \xi, \eta \in \mathbb{S}^{d-1}, \tag{9}$$

we can write

$$I(g) = \int_{\mathbb{S}^{d-1}} g(2^{1/2}(1 - \xi \cdot \eta)^{1/2}) Y_n(\eta) dS^{d-1}(\eta).$$

Applying Theorem 1, we obtain the formula (7) with the coefficient μ_n given by (8).

Using the Rodrigues representation formula (3) for the Legendre polynomial $P_{n,d}(t)$, we can express μ_n from (8) in the form of

$$\mu_n = (-1)^n |\mathbb{S}^{d-2}| R_{n,d} \int_{-1}^1 g(2^{1/2}(1-t)^{1/2}) \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\frac{d-3}{2}} dt. \tag{10}$$

Let us apply Proposition 2 to the following function

$$g(t) = t^\nu, \tag{11}$$

where $\nu \in \mathbb{R}$ is a fixed number. The condition (6) requires

$$\nu > 1 - d. \tag{12}$$

In the following we assume (12) is satisfied. Then from (7) and (10), we have the integral identity

$$\int_{\mathbb{S}^{d-1}} |\xi - \eta|^\nu Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \tag{13}$$

where

$$\mu_n = (-1)^n 2^{\nu/2} |\mathbb{S}^{d-2}| R_{n,d} \int_{-1}^1 (1-t)^{\nu/2} \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\frac{d-3}{2}} dt. \tag{14}$$

We can simplify the formula for μ_n through computing the integral

$$I(\nu) = \int_{-1}^1 (1-t)^{\nu/2} \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\frac{d-3}{2}} dt. \quad (15)$$

Recalling the condition (12), we can perform integration by parts repeated on $I(\nu)$ and all the boundary value terms at $t = \pm 1$ vanish. After integrating by parts n times, we have

$$I(\nu) = \frac{\nu}{2} \left(\frac{\nu}{2} - 1\right) \cdots \left(\frac{\nu}{2} - (n-1)\right) J(\nu), \quad (16)$$

where

$$J(\nu) := \int_{-1}^1 (1-t)^{\nu/2-n} (1-t^2)^{n+\frac{d-3}{2}} dt.$$

Write

$$J(\nu) = \int_{-1}^1 (1-t)^{(\nu+d-3)/2} (1+t)^{n+\frac{d-3}{2}} dt$$

and introduce the change of variables $t = 2s - 1$. Then

$$\begin{aligned} J(\nu) &= 2^{n+\frac{\nu}{2}+d-2} \int_0^1 (1-s)^{\frac{\nu+d-1}{2}-1} s^{n+\frac{d-1}{2}-1} ds \\ &= 2^{n+\frac{\nu}{2}+d-2} \frac{\Gamma\left(\frac{\nu+d-1}{2}\right) \Gamma\left(n+\frac{d-1}{2}\right)}{\Gamma\left(n+\frac{\nu}{2}+d-1\right)}. \end{aligned}$$

Therefore, for μ_n of (14),

$$\mu_n = (-1)^n 2^{\nu+d-1} \pi^{\frac{d-1}{2}} \frac{\nu}{2} \left(\frac{\nu}{2} - 1\right) \cdots \left(\frac{\nu}{2} - (n-1)\right) \frac{\Gamma\left(\frac{\nu+d-1}{2}\right)}{\Gamma\left(n+\frac{\nu}{2}+d-1\right)}. \quad (17)$$

From the formula (17), we see that

$$\mu_n = 0 \quad \text{if } \nu = 0, 2, 4, \dots, 2(n-1).$$

Now consider some special cases for the formula (13) with (17).

Special case 1: $\nu = 2 - d$. Then,

$$\begin{aligned} \mu_n &= 2\pi^{\frac{d-1}{2}} \left(n - 1 + \frac{d-2}{2}\right) \left(n - 2 + \frac{d-2}{2}\right) \cdots \left(1 + \frac{d-2}{2}\right) \frac{d-2}{2} \frac{\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(n + \frac{d}{2}\right)} \\ &= 2\pi^{\frac{d-1}{2}} \frac{\Gamma\left(n + \frac{d-2}{2}\right)}{\Gamma\left(\frac{d-2}{2}\right)} \frac{\pi^{\frac{1}{2}}}{\Gamma\left(n + \frac{d}{2}\right)}. \end{aligned}$$

Use the relations

$$\Gamma\left(n + \frac{d}{2}\right) = \left(n + \frac{d}{2} - 1\right) \Gamma\left(n + \frac{d-2}{2}\right), \quad \Gamma\left(\frac{d-2}{2}\right) = \frac{\Gamma\left(\frac{d}{2}\right)}{\frac{d-2}{2}}.$$

Hence,

$$\mu_n = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)} \frac{d-2}{2n+d-2} = \frac{(d-2)|\mathbb{S}^{d-1}|}{2n+d-2}. \tag{18}$$

So we have the integral identity

$$\int_{\mathbb{S}^{d-1}} \frac{Y_n(\eta)}{|\xi - \eta|^{d-2}} dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \tag{19}$$

where μ_n is given by (18).

Special case 2: $\nu = -1$. Then,

$$\mu_n = 2^{d-2} \pi^{\frac{d-1}{2}} \frac{1}{2} \cdot \frac{3}{2} \cdots \frac{2n-1}{2} \frac{\Gamma\left(\frac{d-2}{2}\right)}{\Gamma\left(n + d - \frac{3}{2}\right)}.$$

After some simplification,

$$\mu_n = 2^{d-2} \pi^{\frac{d-1}{2}} \frac{(2n)!}{2^{2n} n!} \frac{\Gamma\left(\frac{d-2}{2}\right)}{\Gamma\left(n + d - \frac{3}{2}\right)}. \tag{20}$$

So we have the integral identity

$$\int_{\mathbb{S}^{d-1}} \frac{Y_n(\eta)}{|\xi - \eta|} dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \tag{21}$$

where μ_n is given by (20). Note that for $d = 3$,

$$\mu_n = \frac{4\pi}{2n+1}. \tag{22}$$

Special case 3: $\nu = 1$. Then,

$$\mu_n = (-1)^n 2^d \pi^{\frac{d-1}{2}} \frac{1}{2} \left(-\frac{1}{2}\right) \left(-\frac{3}{2}\right) \cdots \left(-\left(n - \frac{3}{2}\right)\right) \frac{\Gamma\left(\frac{d}{2}\right)}{\Gamma\left(n + d - \frac{1}{2}\right)}.$$

Since

$$\Gamma\left(n + d - \frac{1}{2}\right) = \left(n + d - \frac{3}{2}\right) \left(n + d - \frac{5}{2}\right) \cdots \frac{1}{2} \Gamma\left(\frac{1}{2}\right),$$

we have

$$\mu_n = -2^{2d-1} \pi^{\frac{d-2}{2}} \frac{\Gamma\left(\frac{d}{2}\right)}{(2n-1)(2n+1)\cdots(2n+2d-3)}. \quad (23)$$

So we have the integral identity

$$\int_{\mathbb{S}^{d-1}} |\xi - \eta| Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \quad (24)$$

where μ_n is given by (23). Note that for $d = 3$,

$$\mu_n = -\frac{16\pi}{(2n-1)(2n+1)(2n+3)}. \quad (25)$$

We may also choose g as a log function in applying Proposition 2:

$$g(t) = \log t.$$

Then we obtain the formula

$$\int_{\mathbb{S}^{d-1}} \log |\xi - \eta| Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \quad (26)$$

where

$$\mu_n = \frac{|\mathbb{S}^{d-2}|}{2} \int_{-1}^1 \log(2(1-t)) P_{n,d}(t) (1-t^2)^{\frac{d-3}{2}} dt. \quad (27)$$

Using the orthogonality of the Legendre polynomials, for $n \geq 1$, we can simplify (27) to

$$\mu_n = \frac{|\mathbb{S}^{d-2}|}{2} \int_{-1}^1 \log(1-t) P_{n,d}(t) (1-t^2)^{\frac{d-3}{2}} dt, \quad n \geq 1. \quad (28)$$

3 Some extensions

Proposition 2 can be extended straightforward to some other similar integrals.

Let a and b be non-zero real numbers. Then similar to (9),

$$|a \xi + b \eta| = \left(a^2 + b^2 + 2 a b \xi \cdot \eta \right)^{1/2}, \quad \xi, \eta \in \mathbb{S}^{d-1}. \tag{29}$$

Then for a function g satisfying

$$g\left((a^2 + b^2 + 2 a b t)^{1/2} \right) \in L^1_{(d-3)/2}(-1, 1),$$

we can apply Theorem 1 to get

$$\int_{\mathbb{S}^{d-1}} g(|a \xi + b \eta|) Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \tag{30}$$

where

$$\mu_n = (-1)^n |\mathbb{S}^{d-2}| R_{n,d} \int_{-1}^1 g\left((a^2 + b^2 + 2 a b t)^{1/2} \right) \left(\frac{d}{dt} \right)^n (1 - t^2)^{n + \frac{d-3}{2}} dt. \tag{31}$$

This formula includes Proposition 2 as a special case where $a = 1, b = -1$. Choosing $a = b = 1$, we obtain another special case formula:

$$\int_{\mathbb{S}^{d-1}} g(|\xi + \eta|) Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \tag{32}$$

where

$$\mu_n = (-1)^n |\mathbb{S}^{d-2}| R_{n,d} \int_{-1}^1 g(2^{1/2}(1 + t)^{1/2}) \left(\frac{d}{dt} \right)^n (1 - t^2)^{n + \frac{d-3}{2}} dt. \tag{33}$$

More generally, let $g(t_1, \dots, t_L)$ be a function of L real variables, and let $a_l, b_l, 1 \leq l \leq L$, be $2L$ non-zero real numbers. Assume

$$g\left((a_1^2 + b_1^2 + 2 a_1 b_1 t)^{1/2}, \dots, (a_L^2 + b_L^2 + 2 a_L b_L t)^{1/2} \right) \in L^1_{(d-3)/2}(-1, 1).$$

Then

$$\int_{\mathbb{S}^{d-1}} g(|a_1 \xi + b_1 \eta|, \dots, |a_L \xi + b_L \eta|) Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \tag{34}$$

where

$$\mu_n = (-1)^n |\mathbb{S}^{d-2}| R_{n,d} \int_{-1}^1 g\left((a_1^2 + b_1^2 + 2a_1b_1t)^{1/2}, \dots, (a_L^2 + b_L^2 + 2a_Lb_Lt)^{1/2}\right) \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\frac{d-3}{2}} dt. \quad (35)$$

As a particular example, for $\nu_1 > 1 - d$ and $\nu_2 > 1 - d$,

$$\int_{\mathbb{S}^{d-1}} |\xi - \eta|^{\nu_1} |\xi + \eta|^{\nu_2} Y_n(\eta) dS^{d-1}(\eta) = \mu_n Y_n(\xi), \quad \xi \in \mathbb{S}^{d-1}, \quad (36)$$

where

$$\mu_n = (-1)^n 2^{(\nu_1+\nu_2)/2} |\mathbb{S}^{d-2}| R_{n,d} \int_{-1}^1 (1-t)^{\nu_1/2} (1+t)^{\nu_2/2} \left(\frac{d}{dt}\right)^n (1-t^2)^{n+\frac{d-3}{2}} dt. \quad (37)$$

4 Conclusion

Applying the Funk-Hecke formula, we have derived identities for some integrals involving spherical harmonics over the unit sphere in an arbitrary dimension. Integral identities of the forms (13) and (26) are useful in numerical approximations of boundary integral equations ([2]). Note that direct derivation of such identities as (19), (21), and (24) are quite involved, often using some form of Green's integral identities (see, e.g., [9]).

Acknowledgments The work of W. Han was partially supported by a grant from the Simons Foundation. The work of H. Zheng was partially supported by The Natural Science Foundation of Zhejiang Province (Y4110077) and The Qianjiang Program Foundation of Zhejiang Province (2011R10054).

References

1. V. Aquilanti, S. Cavalli, C. Coletti, The d -dimensional hydrogen atom: hyperspherical harmonics as momentum space orbitals and alternative Sturmian basis sets. *Chem. Phys.* **214**, 1–13 (1997)
2. K. Atkinson, *The Numerical Solution of Integral Equations of the Second Kind* (Cambridge University Press, UK, 1997)
3. J. Avery, J. Avery, The generalized Sturmian method for calculating spectra of atoms and ions. *J. Math. Chem.* **33**, 145–162 (2003)
4. J. Avery, *Hyperspherical Harmonics; Applications in Quantum Theory* (Kluwer Academic Publishers, Dordrecht, 1989)
5. J. Avery, Selected application of hyperspherical harmonics in quantum theory. *J. Phys. Chem.* **97**, 2406–2412 (1993)
6. J. Avery, *Hyperspherical Harmonics and Generalised Sturmians* (Kluwer Academic Publishers, Dordrecht, 2000)

7. G.-J. Kroes, M.F. Somers, Six-dimensional dynamics of dissociative chemisorption of H_2 on metal surfaces. *J. Theor. Comput. Chem.* **4**, 493–581 (2005)
8. A.V. Meremianin, Hyperspherical harmonics with arbitrary arguments. *J. Math. Phys.* **50**, 013526 (2009)
9. S.G. Mikhlin, *Mathematical Physics: An Advanced Course* (North-Holland, Amsterdam, 1970)
10. C. Müller, *Analysis of Spherical Symmetries in Euclidean Spaces* (Springer, Berlin, 1998)
11. X.-G. Wang, T. Carrington Jr, Six-dimensional variational calculation of the bending energy levels of HF trimer and DF trimer. *J. Chem. Phys.* **115**, 9781–9796 (2001)
12. R.J. Yáñez, W. Van Assche, R. González-Férez, J.S. Dehesa, Entropic integrals of hyperspherical harmonics and spatial entropy of D -dimensional central potentials. *J. Math. Phys.* **40**, 5675–5686 (1999)