Enseñanza *Revista Mexicana de Física* **41**, *No. 1 (1995) 139–146*

Rotation matrices and spherical harmonics

G.F. TORRES DEL CASTILLO
Departamento de Física Matemática, Instituto de Ciencias
Universidad Autónoma de Puebla, 72000 Puebla, Pue., México

AND

A. HERNÁNDEZ GUEVARA
Facultad de Ciencias Físico Matemáticas, Universidad Autónoma de Puebla
Apartado postal 1152, Puebla, Pue., México

Recibido el 18 de mayo de 1994; aceptado el 2 de diciembre de 1994

ABSTRACT. Making use of the action of the rotation group SO(3) on the sphere, the Wigner D-functions are expressed in terms of the spherical harmonics and of the spin-weighted spherical harmonics.

RESUMEN. Usando la acción del grupo de rotaciones SO(3) sobre la esfera, las funciones D de Wigner se expresan en términos de los armónicos esféricos y de los armónicos esféricos con peso de espín.

PACS: 02.20.Qs; 02.30.Gp

1. INTRODUCTION

As is well known, the ordinary spherical harmonics of order l, Y_{lm} ($m = 0, \pm 1, \ldots, \pm l$), form a basis for a unitary irreducible representation of the rotation group SO(3). The corresponding matrix elements —known as generalized spherical functions, Wigner functions or D-functions— can be calculated making use of the homomorphism of SU(2) onto SO(3) (see, *e.g.*, Refs. [1,2]).

In this paper we find an expression for the generalized spherical functions making use of the action of SO(3) on the sphere. The procedure followed here is applicable to find representations of other Lie groups and in Ref. [3] it has been employed in the case of the group of rigid motions on the plane. In Sect. 2 we show that if SO(3) is parametrized by Euler angles, the generalized spherical functions can be written in terms of the spherical harmonics. In Sect. 3, we show that the generalized spherical functions are also related to the spin-weighted spherical harmonics [4–6]; this relationship was previously established in Ref. [2] by comparing the explicit expressions of both functions.

2. THE ROTATION MATRICES

The ordinary spherical harmonics, Y_{lm}, are functions defined on the sphere that form bases for representations of SO(3). Indeed, taking into account the fact that the cartesian components of the angular momentum operator, $\mathbf{L} = -i\mathbf{r} \times \nabla$, are infinitesimal generators of rotations about the coordinate axes, the relations

$$\begin{aligned} L_3 Y_{lm} &= m\, Y_{lm}, \\ L_\pm Y_{lm} &= \sqrt{l(l+1) - m(m \pm 1)}\; Y_{l,m\pm 1}, \end{aligned} \tag{1}$$

where $L_\pm \equiv L_1 \pm iL_2$, signify that under any rotation, the function Y_{lm} transforms into a linear combination of spherical harmonics of the same order l.

Alternatively, using that Y_{lm} is an eigenfunction of L^2 with eigenvalue $l(l+1)$:

$$L^2 Y_{lm} = l(l+1)\, Y_{lm}, \tag{2}$$

and that the operator L^2 is invariant under rotations (which can be deduced from the fact that L^2 commutes with the components of $\mathbf{L}$) it follows that if $R \in \mathrm{SO}(3)$ and $R\,Y_{lm}$ denotes the result of rotating the function Y_{lm} by means of R,

$$[R\,Y_{lm}](\mathbf{r}) \equiv Y_{lm}(R^{-1}(\mathbf{r})), \tag{3}$$

then $R\,Y_{lm}$ is also an eigenfunction of L^2 with eigenvalue $l(l+1)$; hence,

$$R\,Y_{lm} = \sum_{m'=-l}^{l} D^l_{m'm}(R)\; Y_{lm'}, \tag{4}$$

where $D^l_{m'm}(R)$ are complex numbers that depend on R. For a fixed l, the matrices of order $2l+1$ with elements $D^l_{m'm}(R)$ $(m', m = 0, \pm 1, \ldots, \pm l)$ form a representation of $\mathrm{SO}(3)$ in the sense that

$$D^l_{m'm}(R_1 R_2) = \sum_{r=-l}^{l} D^l_{m'r}(R_1)\; D^l_{rm}(R_2), \tag{5}$$

which follows from Eqs. (3–4). The functions $D^l_{m'm} : \mathrm{SO}(3) \to \mathbf{C}$ are called generalized spherical functions, Wigner functions or D-functions.

The expression

$$(f, g) \equiv \int_0^{2\pi} \int_0^{\pi} \overline{f(\theta, \phi)}\; g(\theta, \phi) \sin\theta \, d\theta \, d\phi, \tag{6}$$

where θ, ϕ are the usual spherical coordinates and the bar denotes complex conjugation, defines an inner product for the complex-valued functions defined on the sphere. The invariance of the solid angle element $\sin\theta\, d\theta\, d\phi$ under rotations implies that

$$(Rf, Rg) = (f, g). \tag{7}$$

Then, the orthonormality of the spherical harmonics, $(Y_{lm}, Y_{l'm'}) = \delta_{ll'}\delta_{mm'}$, and Eqs. (4) and (7) imply that the representation $(D^l_{m'm})$ is unitary:

$$D^l_{m'm}(R^{-1}) = \overline{D^l_{mm'}(R)}, \tag{8}$$

and using Eqs. (4–5) and (8) one finds that

$$\sum_{m=-l}^{l} \overline{[R\,Y_{lm}](\theta_1, \phi_1)}\,[R\,Y_{lm}](\theta_2, \phi_2) = \sum_{m=-l}^{l} \overline{Y_{lm}(\theta_1, \phi_1)}\,Y_{lm}(\theta_2, \phi_2), \tag{9}$$

for any $R \in \mathrm{SO}(3)$.

The rotation group will be parametrized by Euler angles in the following manner. Given a system of cartesian coordinates in $\mathbf{R}^3$, we shall denote by $R(\alpha, \beta, \gamma)$ the rotation obtained by composing a rotation about the z axis through an angle α, followed by a rotation through an angle β about the resulting y' axis, and finally by a rotation about the new z'' axis through an angle γ. Thus, with respect to a fixed system of coordinates, under the rotation $R(\alpha, \beta, \gamma)$, a point of the sphere with coordinates (θ, ϕ) is mapped into a point with coordinates (θ', ϕ') given by

$$\begin{aligned}\theta' &= \arccos[\cos\beta\cos\theta - \sin\beta\sin\theta\cos(\phi + \gamma)],\\ \phi' &= \alpha + \arctan\left[\frac{\sin\theta\sin(\phi+\gamma)}{\cos\beta\sin\theta\cos(\phi+\gamma) + \sin\beta\cos\theta}\right],\end{aligned} \tag{10}$$

therefore, using the fact that $[R(\alpha, \beta, \gamma)]^{-1} = R(-\gamma, -\beta, -\alpha)$ and Eq. (3), for a function f defined on the sphere

$$\begin{aligned}[R(\alpha, \beta, \gamma)f](\theta, \phi) = f\Big(&\arccos(\cos\beta\cos\theta + \sin\beta\sin\theta\cos(\phi - \alpha)),\\ &-\gamma + \arctan\left[\frac{\sin\theta\sin(\phi-\alpha)}{\cos\beta\sin\theta\cos(\phi-\alpha) - \sin\beta\cos\theta}\right]\Big).\end{aligned} \tag{11}$$

Since $Y_{lm}(0, \phi) = [(2l+1)/4\pi]^{1/2}\delta_{m0}$, Eq. (9) applied to $R = R(\phi_1, \theta_1, \gamma)$ yields

$$[R(\phi_1, \theta_1, \gamma)\,Y_{l0}](\theta_2, \phi_2) = \left[\frac{4\pi}{2l+1}\right]^{1/2} \sum_{m=-l}^{l} \overline{Y_{lm}(\theta_1, \phi_1)}\,Y_{lm}(\theta_2, \phi_2). \tag{12}$$

By comparing Eq. (12) with Eq. (4) one finds that

$$D^l_{m'0}(\alpha, \beta, \gamma) = \left[\frac{4\pi}{2l+1}\right]^{1/2} \overline{Y_{lm'}(\beta, \alpha)}, \tag{13}$$

where, as in what follows, $D^l_{m'm}(\alpha,\beta,\gamma) \equiv D^l_{m'm}(R(\alpha,\beta,\gamma))$. Taking into account that $Y_{l0}(\theta,\phi) = [(2l+1)/4\pi]^{1/2} P_l(\cos\theta)$, from Eqs. (11–12) one obtains the addition theorem of spherical harmonics

$$P_l(\cos\Theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} \overline{Y_{lm}(\theta_1,\phi_1)}\, Y_{lm}(\theta_2,\phi_2), \tag{14}$$

where $\cos\Theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_2 - \phi_1)$.

Using Eq. (11) and the chain rule one finds that the angular momentum operators

$$L_\pm = e^{\pm i\phi}(\pm\partial_\theta + i\cot\theta\,\partial_\phi), \qquad L_3 = -i\partial_\phi, \tag{15}$$

satisfy the identities

$$\begin{aligned} i\partial_\gamma[R(\alpha,\beta,\gamma)f] &= R(\alpha,\beta,\gamma)(-i\partial_\phi f), \\ -e^{\mp i\gamma}(\pm\partial_\beta + i\csc\beta\,\partial_\alpha - i\cot\beta\,\partial_\gamma)[R(\alpha,\beta,\gamma)f] &= R(\alpha,\beta,\gamma)[e^{\pm i\phi}(\pm\partial_\theta + i\cot\theta\,\partial_\phi)f], \end{aligned} \tag{16}$$

which relate the action of SO(3) on itself with its action on the sphere. Among other things, these equations imply that the operators

$$M_\pm \equiv -e^{\mp i\gamma}(\pm\partial_\beta + i\csc\beta\,\partial_\alpha - i\cot\beta\,\partial_\gamma), \qquad M_3 \equiv i\partial_\gamma, \tag{17}$$

satisfy the same commutation relations as $L_\pm$ and L_3, namely,

$$[M_3, M_\pm] = \pm M_\pm, \qquad [M_+, M_-] = 2M_3, \tag{18}$$

as can also be verified by a direct computation using the explicit expressions (17).

By applying M_3 and $M_\pm$ to both sides of Eq. (4), making use of Eqs. (1), (4) and (16), one obtains

$$M_3 D^l_{m'm} = m\, D^l_{m'm}, \tag{19}$$

$$M_\pm D^l_{m'm} = \sqrt{l(l+1) - m(m\pm1)}\, D^l_{m',m\pm1} \tag{20}$$

(*cf.* Eqs. (23) of Ref. [3]). Equation (20) implies that

$$D^l_{m'm} = \left[\frac{(l-m)!}{(l+m)!}\right]^{1/2} (M_+)^m D^l_{m'0}, \qquad m > 0,$$

therefore, using Eqs. (13) and (17),

$$D^l_{m'm}(\alpha,\beta,\gamma) = \left[\frac{4\pi}{2l+1}\frac{(l-m)!}{(l+m)!}\right]^{1/2} \overline{(-M_-)^m Y_{lm'}(\beta,\alpha)}, \qquad m > 0. \tag{21}$$

For a function f that does not depend on γ, from Eq. (17) we see that

$$\begin{aligned}(-M_-)^2 f &= e^{i\gamma}(-\partial_\beta + i\csc\beta\,\partial_\alpha - i\cot\beta\,\partial_\gamma)e^{i\gamma}(-\partial_\beta + i\csc\beta\,\partial_\alpha)f \\ &= e^{i\gamma}[e^{i\gamma}(-\partial_\beta + i\csc\beta\,\partial_\alpha)(-\partial_\beta + i\csc\beta\,\partial_\alpha)f + e^{i\gamma}\cot\beta(-\partial_\beta + i\csc\beta\,\partial_\alpha)f] \\ &= e^{2i\gamma}[(-\partial_\beta + i\csc\beta\,\partial_\alpha + \cot\beta)(-\partial_\beta + i\csc\beta\,\partial_\alpha)f] \\ &= e^{2i\gamma}[\sin\beta(-\partial_\beta + i\csc\beta\,\partial_\alpha)\frac{1}{\sin\beta}(-\partial_\beta + i\csc\beta\,\partial_\alpha)f] \\ &= e^{2i\gamma}\sin^2\beta\left[-\frac{1}{\sin\beta}(\partial_\beta - \frac{i}{\sin\beta}\partial_\alpha)\right]^2 f\end{aligned}$$

and, in a similar manner,

$$(-M_-)^m f = e^{im\gamma}\sin^m\beta\left[-\frac{1}{\sin\beta}(\partial_\beta - \frac{i}{\sin\beta}\partial_\alpha)\right]^m f,$$

thus, since $Y_{lm'}(\beta,\alpha)$ does not depend on γ, using Eq. (21) we can write, for $m > 0$,

$$D^l_{m'm}(\alpha,\beta,\gamma) = \left[\frac{4\pi}{2l+1}\frac{(l-m)!}{(l+m)!}\right]^{1/2}\overline{e^{im\gamma}\sin^m\beta\left[-\frac{1}{\sin\beta}(\partial_\beta - \frac{i}{\sin\beta}\partial_\alpha)\right]^m Y_{lm'}(\beta,\alpha)}. \tag{22}$$

Similarly, from Eqs. (13), (17) and (20) it follows that, for $m < 0$,

$$\begin{aligned}D^l_{m'm}(\alpha,\beta,\gamma) &= \left[\frac{(l+m)!}{(l-m)!}\right]^{1/2}(M_-)^{-m}D^l_{m'0} \\ &= \left[\frac{4\pi}{2l+1}\frac{(l+m)!}{(l-m)!}\right]^{1/2}\overline{(-M_+)^{-m}Y_{lm'}(\alpha,\beta)} \\ &= \left[\frac{4\pi}{2l+1}\frac{(l+m)!}{(l-m)!}\right]^{1/2}\overline{e^{im\gamma}\sin^{-m}\beta\left[\frac{1}{\sin\beta}(\partial_\beta + \frac{i}{\sin\beta}\partial_\alpha)\right]^{-m} Y_{lm'}(\beta,\alpha)}.\end{aligned} \tag{23}$$

Equations (22–23), together with the relation $\overline{Y_{lm}} = (-1)^m Y_{l,-m}$, imply that the D-functions satisfy the relation

$$\overline{D^l_{m'm}} = (-1)^{m+m'}D^l_{-m',-m}, \tag{24}$$

and using the fact that $Y_{l0}(\beta,\alpha) = [(2l+1)/4\pi]^{1/2}P_l(\cos\beta)$ does not depend on α, Eqs. (22–23) give

$$D^l_{0m}(\alpha,\beta,\gamma) = (-1)^m\left[\frac{4\pi}{2l+1}\right]^{1/2}\overline{Y_{lm}(\beta,\gamma)}. \tag{25}$$

Since $[R(\alpha,\beta,\gamma)]^{-1} = R(-\gamma,-\beta,-\alpha)$, Eq. (8) amounts to

$$D^l_{m'm}(-\gamma,-\beta,-\alpha) = \overline{D^l_{mm'}(\alpha,\beta,\gamma)}. \tag{26}$$

Thus, taking the complex conjugate of Eqs. (19–20) and replacing (α,β,γ) by $(-\gamma,-\beta,-\alpha)$ one gets

$$\begin{aligned} K_3 D^l_{m'm} &= m' D^l_{m'm}, \\ K_\pm D^l_{m'm} &= \sqrt{l(l+1) - m'(m'\pm 1)}\, D^l_{m'\pm 1,m}, \end{aligned} \tag{27}$$

where (*cf.* Eqs. (17))

$$K_\pm \equiv e^{\mp i\alpha}(\pm\partial_\beta + i\csc\beta\,\partial_\gamma - i\cot\beta\,\partial_\alpha), \qquad K_3 \equiv i\partial_\alpha. \tag{28}$$

Since $K_\pm$ and K_3 are obtained by taking the complex conjugate of $M_\pm$ and M_3, substituting (α,β,γ) by $(-\gamma,-\beta,-\alpha)$, the operators $K_\pm$ and K_3 also obey the commutation relations (18),

$$[K_3, K_\pm] = \pm K_\pm, \qquad [K_+, K_-] = 2K_3. \tag{29}$$

Furthermore, one finds that

$$[M_i, K_j] = 0, \qquad i,j = 1,2,3, \tag{30}$$

where

$$M_\pm \equiv M_1 \pm iM_2, \qquad K_\pm \equiv K_1 \mp iK_2. \tag{31}$$

From Eqs. (19–20) and (27) it follows that

$$M^2 D^l_{m'm} = K^2 D^l_{m'm} = l(l+1) D^l_{m'm}, \tag{32}$$

where $M^2 = {M_1}^2 + {M_2}^2 + {M_3}^2 = M_-M_+ + {M_3}^2 + M_3$ and $K^2 = {K_1}^2 + {K_2}^2 + {K_3}^2 = K_-K_+ + {K_3}^2 + K_3$. In fact,

$$M^2 = K^2 = -\left\{\frac{1}{\sin\beta}\partial_\beta(\sin\beta\,\partial_\beta) + \frac{1}{\sin^2\beta}(\partial_\alpha^2 - 2\cos\beta\,\partial_\alpha\partial_\gamma + \partial_\gamma^2)\right\}. \tag{33}$$

The operators M_i and K_i also arise in the study of the symmetric top in quantum mechanics; except for a constant factor, they correspond to the components of the angular momentum of a rigid body with respect to the body axes and to the space axes, respectively (see, *e.g.*, Ref. [7]; note, however, that Eqs. (28) and (33) differ from Eqs. (44.28–29) of Ref. [7] and our expressions (17) and (28) are not equivalent to Eqs. (3.18) and (3.16) of Ref. [2], despite the fact that in all cases the rotations are parametrized in the same form.)

3. RELATIONSHIP WITH THE SPIN-WEIGHTED SPHERICAL HARMONICS

The spin-weighted spherical harmonics [4–6], ${}_sY_{lm}$, can be defined by

$$
{}_sY_{lm}(\theta,\phi) \equiv \begin{cases} \left[\frac{(l-s)!}{(l+s)!}\right]^{1/2} \sin^s\theta \left[-\frac{1}{\sin\theta}(\partial_\theta + \frac{i}{\sin\theta}\partial_\phi)\right]^s Y_{lm}(\theta,\phi), & s \geq 0, \\ \left[\frac{(l+s)!}{(l-s)!}\right]^{1/2} \sin^{-s}\theta \left[\frac{1}{\sin\theta}(\partial_\theta - \frac{i}{\sin\theta}\partial_\phi)\right]^{-s} Y_{lm}(\theta,\phi), & s \leq 0, \end{cases} \tag{34}
$$

(the factor $[(l-|s|)!/(l+|s|)!]^{1/2}$ is a normalization factor such that $({}_sY_{lm}, {}_sY_{l'm'}) = \delta_{ll'}\delta_{mm'}$). The spin-weighted spherical harmonics are very useful in the solution of non-scalar partial differential equations (see, *e.g.*, Refs. [2,8–10]). Comparison of Eqs. (22–23) with Eq. (34) yields

$$
D^l_{m'm}(\alpha,\beta,\gamma) = (-1)^m \left[\frac{4\pi}{2l+1}\right]^{1/2} \overline{e^{im\gamma}{}_{-m}Y_{lm'}(\beta,\alpha)} \tag{35}
$$

or, equivalently, owing to Eq. (26)

$$
D^l_{mm'}(-\gamma,-\beta,-\alpha) = (-1)^m \left[\frac{4\pi}{2l+1}\right]^{1/2} e^{im\gamma}{}_{-m}Y_{lm'}(\beta,\alpha). \tag{36}
$$

A relationship equivalent to Eq. (36) was obtained in Ref. [2] by comparing the explicit expressions of the D-functions and of the spin-weighted spherical harmonics.

Equation (35) enables us to derive some properties of the spin-weighted spherical harmonics. (*Cf.* also Ref. [2]. Note, however, that Eqs. (2.7a), (3.10) and (3.18–20) of Ref. [2] are not consistent.) For example, substituting Eq. (35) into the complex conjugates of Eqs. (27), using the fact that $\overline{K_\pm} = -K_\mp$ and making some obvious changes of indices, we get

$$
\begin{aligned}
-i\partial_\alpha\, {}_sY_{lm}(\beta,\alpha) &= m\, {}_sY_{lm}(\beta,\alpha), \\
e^{\pm i\alpha}(\pm\partial_\beta + i\cot\beta\,\partial_\alpha - \frac{s}{\sin\beta})\,{}_sY_{lm}(\beta,\alpha) &= \sqrt{l(l+1)-m(m\pm1)}\,{}_sY_{l,m\pm1}(\beta,\alpha)
\end{aligned} \tag{37}
$$

(*cf.* Eqs. (1)). (The operators appearing in Eqs. (37) are given in Ref. [11] and, as shown in Refs. [9,10], these operators correspond to total angular momentum.)

In a similar manner, one finds that Eqs. (19–20) are equivalent to

$$
-(\partial_\beta \pm \frac{i}{\sin\beta}\partial_\beta \mp s\cot\beta)\,{}_sY_{lm}(\beta,\alpha) = \pm\sqrt{l(l+1)-s(s\pm1)}\,{}_{s\pm1}Y_{lm}(\beta,\alpha). \tag{38}
$$

(The operators acting on ${}_sY_{lm}$ in the left-hand side of Eq. (38) are denoted as $\eth$ and $\overline{\eth}$ in Refs. [2,4,6].)

Finally, substituting Eq. (35) into Eq. (4) one obtains the formula

$$Y_{lm}(\Theta, \Phi) = (-1)^m \left[\frac{4\pi}{2l+1}\right]^{1/2} \sum_{m'=-l}^{l} \overline{{}_{-m}Y_{lm'}(\theta_1, \phi_1)}\, Y_{lm'}(\theta_2, \phi_2), \tag{39}$$

where $\cos\Theta = \cos\theta_1 \cos\theta_2 + \sin\theta_1 \sin\theta_2 \cos(\phi_2 - \phi_1)$, $\tan\Phi = (\sin\theta_2 \sin(\phi_2 - \phi_1))/(\cos\theta_1 \sin\theta_2 \cos(\phi_2 - \phi_1) - \sin\theta_1 \cos\theta_2)$, which is analogous to Neumann's addition theorem for Bessel functions and reduces to Eq. (14) when $m = 0$.

4. Concluding remarks

The relations (16), based on the action of SO(3) on the sphere, together with the choice of the ordinary spherical harmonics as bases for representations of SO(3), lead to the basic formulae (19–20), which allow us to obtain expressions (22–23) for the rotation matrices. A similar procedure can be used to find representations of the isometry groups of other manifolds and to derive addition theorems analogous to Eq. (14) (see, *e.g.*, Refs. [3,12]). (Note that SO(3) is the group of the orientation-preserving isometries of the sphere and that the spherical harmonics are the regular eigenfunctions of $-L^2$, which is the Laplace operator on the sphere.) It may be noticed that the validity of Eqs. (27) follows from that of Eqs. (19–20) owing to the simple relation between the Euler angles of R^{-1} and those of R.

Acknowledgment

This work was supported in part by CONACYT.

References

1. E.P. Wigner, *Group Theory and Its Applications to the Quantum Mechanics of Atomic Spectra*, Academic Press, New York (1959).
2. J.N. Goldberg, A.J. Macfarlane, E.T. Newman, F. Rohrlich, and E.C.G. Sudarshan, *J. Math. Phys.* **8** (1967) 2155.
3. G.F. Torres del Castillo, *J. Math. Phys.* **34** (1993) 3856.
4. E. Newman and R. Penrose, *J. Math. Phys.* **7** (1966) 863.
5. R. Penrose and W. Rindler, *Spinors and Space-time*, Vol. 1, Cambridge University Press, Cambridge (1984).
6. G.F. Torres del Castillo, *Rev. Mex. Fís.* **36** (1990) 446. (In Spanish.)
7. A.S. Davydov, *Quantum Mechanics*, 2nd ed., Pergamon, Oxford (1988).
8. G.F. Torres del Castillo, *J. Math. Phys.* **35** (1994) 499.
9. G.F. Torres del Castillo, *Rev. Mex. Fís.* **37** (1991) 147. (In Spanish.)
10. G.F. Torres del Castillo and C. Uribe Estrada, *Rev. Mex. Fís.* **38** (1992) 162. (In Spanish.).
11. T. Dray, *J. Math. Phys.* **26** (1985) 1030.
12. A. Hernández Guevara, Tesis de Licenciatura, UAP, 1995.