Representations of the full rotation group

In this section, we will describe the odd-dimensional irreducible representations of the full proper rotation group in 3 dimensions ($SO(3)$), and show that the spherical harmonics represent a particularly useful basis set for functions on the surface of a unit sphere. Here, the operator g will represent a *proper rotation*.

Once again, let's recall our definition of symmetry transformations for functions and their gradients:

$$
\begin{aligned}
g[f(\boldsymbol{x})] &= f(\boldsymbol{R}^{-1}(g)\boldsymbol{x}) && (1)\\
g[\boldsymbol{\nabla} f(\boldsymbol{x})] &= (\boldsymbol{R}(g)\boldsymbol{\nabla})\, f(\boldsymbol{R}^{-1}(g)\boldsymbol{x}) && (2)
\end{aligned}
$$

Eq. 1 and 2 can be generalised to any coordinate set, including spherical coordinates. The important points are

- We are employing *active* transformations, so we are **not** changing the coordinate system.
- The way eq. 1 is to be interpreted is therefore the following: the *transformed* (e.g., rotated) function $g[f(\boldsymbol{x})]$ is a new function of the *original* variables, obtained by replacing the *formal* variables in $f(\boldsymbol{x})$ with new values describing the position of a back-transformed point.

We can therefore generalise eq. 1 to spherical coordinates as

$$g[f(r,\theta,\phi)] = f(r,\tilde{\theta}(\theta,\phi),\tilde{\phi}(\theta,\phi)) \quad (3)$$

where, once again, $\tilde{\theta}(\theta,\phi)$ and $\tilde{\phi}(\theta,\phi)$ are the angular coordinate of a point that has been back-rotated with respect to the point r,θ,ϕ. Clearly, the expression of $\tilde{\theta}(\theta,\phi)$ and $\tilde{\phi}(\theta,\phi)$ as a function of their arguments depends on the magnitude and on the direction of rotation, as expressed, for example, through the Euler angles (we are not concerned with the exact expression here).

We aim to show that

1. The spherical harmonics $Y_l^m(\theta,\phi)$ are basis functions of an irreducible $2l+1$-dimensional space.
2. On the basis of the spherical harmonics, rotations are represented by $(2l+1)\times(2l+1)$ matrices, known as the Wigner D-matrices.

In order to show this, we recall that the spherical harmonics are the solutions of the angular part of the Laplace equation $\nabla^2\psi(r,\theta,\phi) = 0$. In quantum mechanics, they are also thought as the angular part of the (common) eigenvectors of the operators $\hat{\boldsymbol{L}}^2$ and $\hat{L}_z$. It can be shown that the two definitions are equivalent, since the spherical harmonics are eigenfunction of the operator:

$$
\begin{aligned}
\frac{1}{\hbar^2}\hat{\boldsymbol{L}}^2 &= -r^2\nabla^2 + \left(r\frac{\partial}{\partial r} + 1\right) r\frac{\partial}{\partial r} \\
&= -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}
\end{aligned} \tag{4}
$$

with eigenvalue $l(l+1)$. With a suitable choice of basis, these functions are also eigenfunctions of $\hat{L}_z$ with:

$$
\frac{1}{\hbar}\hat{L}_z Y_l^m(\tilde{\theta},\tilde{\phi}) = mY_l^m(\tilde{\theta},\tilde{\phi}) \tag{5}
$$

The crucial observation is that the operator $\hat{\boldsymbol{L}}^2$ is *rotationally invariant* (while $\hat{L}_z$ is not!. This can be seen directly from eq. 4). Therefore, if we apply a rotation to the whole eigenvalue equation we get:

$$
\frac{1}{\hbar^2}\hat{\boldsymbol{L}}^2 Y_l^m(\tilde{\theta},\tilde{\phi}) = \hat{\boldsymbol{L}}^2 Y_l^m(\tilde{\theta},\tilde{\phi}) = l(l+1)Y_l^m(\tilde{\theta},\tilde{\phi}) \tag{6}
$$

In other words, the new function $Y_l^m\left(\tilde{\theta}(\theta,\phi),\tilde{\phi}(\theta,\phi)\right)$, intended as a function of the original coordinates θ,ϕ is *also* a solution of the eigenvalue equation with the *same* eigenvalues, and must necessarily be a linear combination of the degenerate eigenvectors:

$$
T_g[Y_l^m(\theta,\phi)] = Y_l^m\left(\tilde{\theta}(\theta,\phi),\tilde{\phi}(\theta,\phi)\right) = \sum_{m=-l}^{+l} D^l_{mm'}(\alpha\beta\gamma)Y_l^{m'}(\theta,\phi) \tag{7}
$$

where we have introduced the explicit dependence of the matrices $D^l_{mm'}(\alpha\beta\gamma)$ on the Euler angles. Eq. 7 is the very definition of a $2l+1$-dimensional representation of the rotation group $SO(3)$ on the relevant subspace of defined by the $2l+1$ spherical harmonics with a given l. It is also possible to show [**?**] that this representation is *irreducible*. one should also remark that, since the spherical harmonics are a complete set for the linear space of functions on the unit sphere, the full representation decomposes in odd-dimensional irreducible representations only (we will learn about even-dimensional irreducible representations later on).

The matrix elements $D_{lm'}(\alpha\beta\gamma)$ are known as the **Wigner D-matrices**, and have a complicated expression that can be found in [**?**]. The Wigner D-matrices are better known as the matrix elements of the *rotation operator* $\hat{R}(\alpha\beta\gamma)$ on the basis of the spherical harmonics:

$$D^l_{mm'}(\alpha\beta\gamma) = \langle l, m'|\hat{R}(\alpha\beta\gamma)|l, m\rangle \tag{8}$$

We are not concerned here with the explicit form of the $\hat{R}(\alpha\beta\gamma)$, since , for most purposes, it is sufficient to know their *characters*.

The characters can be found as follows: for any rotation, it is always possible to bring the corresponding matrix in diagonal form by choosing as a basis a set of spherical harmonics having the polar axis along the direction of rotation. If this is the case, and if the rotation is on an angle α, then we can re-write eq. 3 as

$$T_{g_\alpha}[Y^m_l(\theta,\phi)] = Y^m_l(\theta,\phi-\alpha) = e^{-im\alpha}Y^m_l(\theta,\phi) \tag{9}$$

where we have used the explicit form of the spherical harmonics:

$$Y^m_l(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P^m_l(\cos\theta)e^{im\phi} \tag{10}$$

The matrix representation in this coordinate system is therefore diagonal and reads

$$\begin{bmatrix} e^{-il\alpha} & & & \\ & e^{-i(l-1)\alpha} & & \\ & & \ddots & \\ & & & e^{+il\alpha} \end{bmatrix} \tag{11}$$

whence, after a simple summation, we can deduce the character:

$$\chi^l(\alpha) = \frac{\sin[(l+\frac{1}{2})\alpha]}{\sin[(\frac{1}{2})\alpha]} \tag{12}$$

Note that

$$
\begin{aligned}
\frac{\sin\frac{3}{2}\alpha}{\sin\frac{1}{2}\alpha} &= \frac{1}{\sin\frac{1}{2}\alpha}\left(\sin\frac{\alpha}{2}\cos\alpha + \cos\frac{\alpha}{2}\sin\alpha\right) \\
&= \frac{1}{\sin\frac{1}{2}\alpha}\left(\sin\frac{\alpha}{2}\cos\alpha + (2\cos^2\frac{\alpha}{2} - 1 + 1)\sin\frac{\alpha}{2}\right) \\
&= 2\cos\alpha + 1 \qquad (13)
\end{aligned}
$$

which is the character of the representation of SO(3) on the ordinary space of 3D vectors (or of linear functions x, y, z). To see this, one can show that a rotation about any axis can always be brought into a rotation about z by a unitary transformation.

We also note for later the explicit form of the *solid harmonics*, which are the solutions of the full Laplace equation, including the radial part:

$$
\begin{aligned}
R_l^m &= \sqrt{\frac{4\pi}{2l+1}} r^l Y_l^m(\theta, \phi) \\
I_l^m &= \sqrt{\frac{4\pi}{2l+1}} r^{-(l+1)} Y_l^m(\theta, \phi) \qquad (14)
\end{aligned}
$$

$R_l^m(r, \theta, \phi)$ and $I_l^m(r, \theta, \phi)$ are known as the *regular* and *irregular* solid harmonics, respectively.

Recursive formula for the characters

We can expand eq. 12 in powers of $\cos\alpha$ to obtain a recursive formula:

$$
\chi^l(\alpha) = \frac{3}{2}\cos l\alpha + \frac{1}{2}\chi^{l-1}(\alpha)(\cos\alpha + 1) + \frac{1}{2}\cos(l-1)\alpha \qquad (15)
$$

to be combined with:

$$
\cos l\alpha = 2\cos\alpha\cos(l-1)\alpha - \cos(l-2)\alpha \qquad (16)
$$

From these, we can obtain the characters of the first four spherical harmonic representations (monopole, dipole, quadrupole and octopole - others are obtained by the same method):

$$
\begin{aligned}
\chi^0(\alpha) &= 1 \\
\chi^1(\alpha) &= 2\cos\alpha + 1 \\
\chi^2(\alpha) &= 4\cos^2\alpha + 2\cos\alpha - 1 \\
\chi^3(\alpha) &= 8\cos^3\alpha + 4\cos^2\alpha - 4\cos\alpha - 1 \qquad (17)
\end{aligned}
$$

The characters of the spin-1/2 rotation representation is easily obtained from the spin rotation matrices, which are given here below as a general formula for a rotation Φ around axis n:

$$R_n(\Phi) = \cos\frac{\Phi}{2}\mathbb{1} - i\sin\frac{\Phi}{2}\sigma_n \tag{18}$$

where σ_n are the Pauli matrices. Therefore, the characters of the $S = \frac{1}{2}$ representation are $\mathrm{Tr}\left(\mathrm{R_n}(\Phi)\right) = 2\cos\frac{\alpha}{2}$ (note that in SO(3) rotation of an angle Φ about any axis are in the same conjugation class, because any axis can be rotated into any other axis). The characters of higher spinor representations are obtained by tensor product with , and iterative subtraction, remembering that the tensor product of a generic L state with a $S = \frac{1}{2}$ reduces to $J = L + \frac{1}{2}$ and $J = L - \frac{1}{2}$. So, for example:

$$\begin{aligned} \chi^{\frac{1}{2}} \otimes \chi^{1} &= (2\cos\alpha + 1)(2\cos\alpha/2) = 4\cos\alpha\cos\alpha/2 + 2\cos\alpha/2 \\ &= \chi^{\frac{1}{2}} + \chi^{\frac{3}{2}} \end{aligned} \tag{19}$$

whence clearly

$$\chi^{\frac{3}{2}}(\alpha) = 4\cos\alpha\cos\alpha/2 \tag{20}$$

More generally

$$\begin{aligned} \chi^{\frac{1}{2}}(\alpha) &= 2\cos\alpha/2 \\ \chi^{\frac{3}{2}}(\alpha) &= 4\cos\alpha\cos\alpha/2 \\ \chi^{\frac{5}{2}}(\alpha) &= \left(8\cos^2\alpha - 2\right)\cos\alpha/2 \\ \chi^{\frac{7}{2}}(\alpha) &= \left(16\cos^3\alpha - 8\cos^2\alpha\right)\cos\alpha/2 \end{aligned} \tag{21}$$

Note that we can also symmetrise and antisymmetrise the tensor products using the usual formula. For example:

$$\begin{aligned} [\chi^1(\alpha) \otimes \chi^1(\alpha)] &= \frac{1}{2}\left((2\cos\alpha + 1)^2 + 2\cos 2\alpha + 1\right) = 4\cos^2\alpha + 2\cos\alpha \\ &= \chi^2(\alpha) + \chi^0(\alpha) \\ \{\chi^1(\alpha) \otimes \chi^1(\alpha)\} &= 2\cos\alpha + 1 = \chi^1(\alpha) \end{aligned} \tag{22}$$

A more complicated example, relevant for the spin Hall effect, is:

$$
\begin{aligned}
[\chi^1(\alpha) \otimes \chi^1(\alpha)] \otimes \chi^1(\alpha) &= 8\cos^3\alpha + 8\cos^2\alpha + 2\cos\alpha \\
&= \chi^3(\alpha) + \chi^2(\alpha) + 2\chi^1(\alpha) \\
\{\chi^1(\alpha) \otimes \chi^1(\alpha)\} \otimes \chi^1(\alpha) &= \chi^2(\alpha) + \chi^1(\alpha) + \chi^0(\alpha) \qquad (23)
\end{aligned}
$$

The hydrogen atom

We recall that the eigenfunctions for the hydrogen atom are:

$$\Psi_{nlm} = R_{nl}(r) Y_l^m(\theta, \phi) \qquad (24)$$

having eigenvalues:

$$E_n = -Ry \frac{1}{n^2} \qquad (25)$$

where Ry is the Rydberg constant and the Bohr radius are (μ is the reduced mass):

$$Ry = \frac{\mu e^4}{8\epsilon_0^2 h^2} \qquad (26)$$

$$a_0 = \frac{4\pi\epsilon_0 \hbar^2}{\mu e^2} \qquad (27)$$

The functions R_{nl} are the hydrogen atom radial functions, which only depend on n and l (not m). From this we can conclude that:

- The hydrogen wavefunctions for a given l and all m and regardless of n form basis functions to the $2l+1$-dimensional irreps of O(3).
- Wavefunctions with a different n also form basis functions.
- Any linear combinations of wavefunctions with different n and the same l, with the same linear combination coefficients for different m as:

$$\psi_{lm} = \sum_n a_n \Psi_{nlm} \qquad (28)$$

are also basis functions for the $2l+1$-dimensional irreps of O(3). Clearly, ψ_{lm} are *not* eigenfunctions of the hydrogen Hamiltonian. All these functions have the same angular part, i.e., the relevant spherical harmonics.

- As it happens, wavefunctions with the same n and different l are degenerate for the hydrogen atom, and consequently any linear combination thereof is a degenerate eigenfunction. This degeneracy is *accidental* in that it is not imposed by symmetry - in fact these wavefunctions are not degenerate for a generic central potential.

Rotation operator and angular momentum

One can show that the unitary operator corresponding to a rotation by an angle α about the z axis can be expressed as:

$$\hat{R}^z_\alpha = e^{-\frac{i}{\hbar}\alpha \hat{l}_z} \tag{29}$$

where $\hat{l}_z$ is the z component of the angular momentum. More generally, any unitary alibi operator can be expressed in the same exponential form with a Hermitian operator. Therefore, if $\hat{R}^z_\alpha$ commutes with the Hamiltonian and α can be made to be infinitesimal, then $\hat{l}_z$ also commute with the Hamiltonian, since

$$\lim_{\alpha \to 0} \hat{R}^z_\alpha = 1 - \frac{i}{\hbar}\alpha \hat{l}_z \tag{30}$$

Therefore, $\hat{l}_z$ represents a conserved physical quantity. Again, in general, anny differentiable continuous symmetry is associated with a conserved quantity (Noether's theorem).