

The Fast Rotation Function

1 The rotation function

Let us consider the patterson function, $P(\mathbf{r})$, for a given structure and the patterson function, $Q(\mathbf{r})$, for a model structure with its centre of mass at the origin of a coordinate system, and having a fixed orientation. The following *overlap function*,

$$\mathcal{R} \equiv \int_S P(\mathbf{r})Q(\mathbf{r})d\mathbf{r},$$

where S is a spherical region of defined radius, centred at the origin, has high values when there is a high overlapping of patterson peaks between the two maps. If the model is rotated, its patterson Q will transform into a new patterson Q' , and the above integral will yield a different value because the overlapping between patterson peaks will have changed.

A rotation can be described by a 3×3 rotation matrix, Ω , which is commonly parametrised using Euler angles or spherical polar angles. A rotated molecular model will have each atomic coordinate (x_j, y_j, z_j) of the original model moved into a new coordinate (x'_j, y'_j, z'_j) given by,

$$\begin{pmatrix} x'_j \\ y'_j \\ z'_j \end{pmatrix} = \Omega \begin{pmatrix} x_j \\ y_j \\ z_j \end{pmatrix}$$

The un-rotated coordinates (x_j, y_j, z_j) can be obtained from the rotated ones simply by using the inverse of the rotation matrix, Ω^{-1} . Therefore, the patterson Q' for the rotated molecule is equivalent to the patterson Q for the un-rotated molecule, where the coordinate system has been rotated with the inverse of Ω :

$$Q'(\mathbf{r}) = Q(\Omega^{-1}\mathbf{r})$$

We can, now, define the *rotation function* starting from the overlap function as,

$$\mathcal{R}(\Omega) \equiv \int_S P(\mathbf{r})Q(\Omega^{-1}\mathbf{r})d\mathbf{r} \quad (1)$$

As stated before, for each rotation (represented by a specific matrix Ω) the overlap integral will yield a different value. High values correspond to a high degree of overlapping between patterson peaks of structure and model, low values to low degree of overlapping. Thus, the rotation function is a map in the three dimensional rotation space, with peaks corresponding to rotations that bring a large number of atoms of the model to match with atoms of the structure. Essentially the rotation stage of a molecular replacement problem consists of computing a rotation function and looking for its peaks, where every one of them corresponds to a rotation potentially aligning the model molecule to the structure.

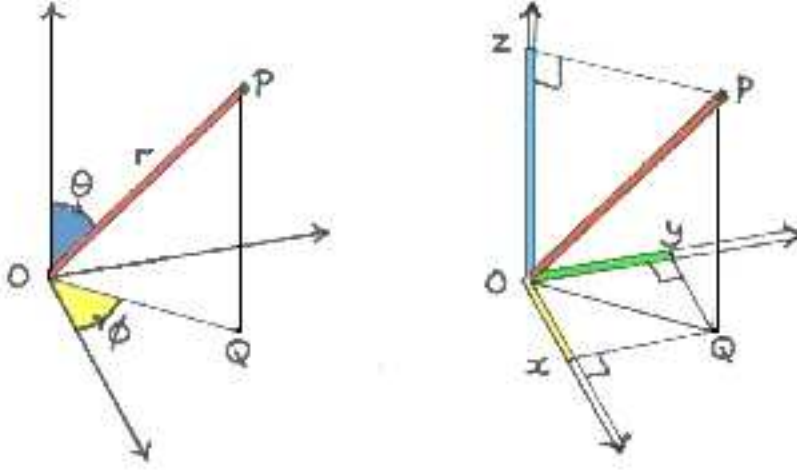


Figure 1: Spherical polar coordinates, (r, θ, ϕ) , and their relation with orthogonal cartesian coordinates; $x = r \sin \theta \cos \phi, y = r \sin \theta \sin \phi, z = r \cos \theta$.

2 Expansion of the fixed patterson in spherical harmonics

The calculation of the rotation function is carried out more naturally using spherical polar coordinates, (r, θ, ϕ) (see Figure 1). Once this system of coordinates is used, functions of θ and ϕ will pop up during the calculations. There is, as a result, the need to expand such functions in an appropriate, complete set of basis functions, themselves depending on θ and ϕ . The *spherical harmonics* are such a set. Like for the well-known fourier series, where any function $f(x, y, z)$ can be expressed as an infinite summation of sines and cosines, any function $f(\theta, \phi)$ can be written as an infinite summation of spherical harmonics. A spherical harmonic function is usually represented by the symbol $Y_\ell^m(\theta, \phi)$, where the integer $\ell = 0, 1, 2, \dots$, while $-\ell \leq m \leq \ell$. These functions form a complete orthonormal set. This means that they obey the following orthonormality condition,

$$\int_0^\pi \int_0^{2\pi} Y_\ell^m(\theta, \phi) Y_{\ell'}^{m'}(\theta, \phi) \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'}, \quad (2)$$

where $\delta_{\ell\ell'}$ and $\delta_{mm'}$ are kronecker symbols. It also means that any well behaved function $f(\theta, \phi)$ can be expanded as,

$$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m} Y_\ell^m(\theta, \phi), \quad (3)$$

where coefficients $a_{\ell m}$ can be computed using the following formula,

$$a_{\ell m} \equiv \int_0^\pi \int_0^{2\pi} f(\theta, \phi) Y_\ell^{m*}(\theta, \phi) \sin \theta d\theta d\phi \quad (4)$$

with $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$. More details on spherical harmonics can be found in Appendix B.

In order to carry out the integration defined at (1) in spherical polar coordinates, and using the expansion in spherical harmonics, one has to start expanding the patterson according to formula (3). This function, though, depends on r , in addition to θ and ϕ . Therefore the expansion coefficients will be functions of r :

$$P(r, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m}(r) Y_\ell^m(\theta, \phi)$$

Let us focus on $a_{\ell m}(r)$. A patterson function is defined as follows:

$$P(\mathbf{r}) \equiv \frac{1}{V} \sum_{\mathbf{s}} |F(\mathbf{s})|^2 \exp(2\pi i \mathbf{s} \cdot \mathbf{r})$$

where $\mathbf{s} \equiv (h, k, l) = (s \sin \theta_s \cos \phi_s, s \sin \theta_s \sin \phi_s, s \cos \theta_s)$ is the position vector in the reciprocal space (s, θ_s and ϕ_s are spherical polar coordinates in the reciprocal lattice), while $\mathbf{r} \equiv (x, y, z) = (r \sin \theta \cos \phi, r \sin \theta \sin \phi, r \cos \theta)$ is the position vector in the direct space. According to (4) $a_{\ell m}(r)$ is defined as,

$$a_{\ell m}(r) = \int_0^\pi \int_0^{2\pi} P(\mathbf{r}) Y_\ell^{m*}(\theta, \phi) \sin \theta d\theta d\phi$$

Therefore,

$$a_{\ell m}(r) = \frac{1}{V} \sum_{\mathbf{s}} |F(\mathbf{s})|^2 \int_0^\pi \int_0^{2\pi} \exp(2\pi i \mathbf{s} \cdot \mathbf{r}) Y_\ell^{m*}(\theta, \phi) \sin \theta d\theta d\phi \quad (5)$$

The above integral can be computed once the following expansion for $\exp(2\pi i \mathbf{s} \cdot \mathbf{r})$ is used:

$$\exp(2\pi i \mathbf{s} \cdot \mathbf{r}) = 4\pi \sum_{\ell=0}^{\infty} i^\ell j_\ell(sr) \sum_{m=-\ell}^{\ell} Y_\ell^{m*}(\theta, \phi) Y_\ell^m(\theta_s, \phi_s), \quad (6)$$

where the $j_\ell(x)$ are *spherical Bessel functions of the first kind* (see Appendix C). The result in (6) can be obtained, for example, using Helmholtz equation and the addition theorem for spherical harmonics. It is normally reported in several textbooks (see for instance [3]). Inserting (6) into (5), and using a simple relation connecting spherical harmonics to their conjugates,

$$Y_\ell^{m*}(\theta, \phi) = (-1)^m Y_\ell^{-m}(\theta, \phi), \quad (7)$$

we obtain:

$$a_{\ell m}(r) = \frac{4\pi}{V} \sum_{\mathbf{s}} |F(\mathbf{s})|^2 \sum_{\ell'=0}^{\infty} i^{\ell'} j_{\ell'}(2\pi sr) \sum_{m'=-\ell'}^{\ell'} (-1)^{m'} Y_{\ell'}^{m'}(\theta_s, \phi_s) \int_0^\pi \int_0^{2\pi} Y_\ell^{m*}(\theta, \phi) Y_{\ell'}^{-m'}(\theta, \phi) \sin \theta d\theta d\phi$$

or, using the orthogonality property (2):

$$\begin{aligned} a_{\ell m}(r) &= \frac{4\pi}{V} \sum_{\mathbf{s}} |F(\mathbf{s})|^2 \sum_{\ell'=0}^{\infty} i^{\ell'} j_{\ell'}(2\pi sr) \sum_{m'=-\ell'}^{\ell'} (-1)^{m'} Y_{\ell'}^{m'}(\theta_s, \phi_s) \delta_{\ell\ell'} \delta_{-m'm} \\ &\quad \downarrow \\ a_{\ell m}(r) &= \frac{4\pi i^\ell}{V} \sum_{\mathbf{s}} |F(\mathbf{s})|^2 j_\ell(2\pi sr) Y_\ell^{m*}(\theta_s, \phi_s) \end{aligned} \quad (8)$$

Quite naturally, given that the patterson was defined as a summation involving structure factors and position vectors in reciprocal space, the coefficients of its spherical harmonics expansion will be given by summations involving structure factors and position vectors in reciprocal space, these last ones in spherical coordinates, (s, θ_s, ϕ_s) .

3 Expansion of the rotated patterson in spherical harmonics. Wigner's theorem

So far we have found the expansion in spherical harmonics for the structure patterson. How about the expansion for the rotated-model patterson, $Q(\Omega^{-1}\mathbf{r})$? First we can expand the unrotated-model patterson in spherical harmonics,

$$Q(r, \theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} b_{\ell m}(r) Y_{\ell}^m(\theta, \phi)$$

This time the expansion coefficients will be computed as,

$$b_{\ell m}(r) = \frac{4\pi i^{\ell}}{V} \sum_{\mathbf{s}} |G(\mathbf{s})|^2 j_{\ell}(2\pi s r) Y_{\ell}^{m*}(\theta_{\mathbf{s}}, \phi_{\mathbf{s}}) \quad (9)$$

with $G(s)$ the calculated structure factors corresponding to the unrotated model. Then we can simply observe that a coordinates rotation Ω^{-1} leaves r unchanged, while transforming θ and ϕ in two new angles θ', ϕ' :

$$Q(\Omega^{-1}\mathbf{r}) = Q(r, \theta', \phi') = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} b_{\ell m}(r) Y_{\ell}^m(\theta', \phi')$$

Thus, the expansion of the rotated patterson in spherical harmonics depends on computing spherical harmonics at modified values of the angles. Wigner [6] has shown that the value of any spherical harmonic at rotated angles (θ', ϕ') is equal to the value of a linear combination of spherical harmonics at unrotated angles, (θ, ϕ) . In formula,

$$Y_{\ell}^m(\theta', \phi') = \sum_{m'=-\ell}^{\ell} D_{m' m}^{\ell}(\Omega^{-1}) Y_{\ell}^{m'}(\theta, \phi) \quad (10)$$

To compute coefficients $D_{m' m}^{\ell}(\Omega^{-1})$ it is convenient to express the rotation operator Ω^{-1} using the Euler angles, (α, β, γ) , corresponding to Ω^{-1} (see for example [2]). In fact Wigner has shown that in this case the coefficients $D_{m' m}^{\ell}(\Omega^{-1}) \equiv D_{m' m}^{\ell}(\alpha, \beta, \gamma)$ can be factorised in the following way,

$$D_{m' m}^{\ell}(\alpha, \beta, \gamma) = \exp(-im'\alpha) d_{m' m}^{\ell}(\beta) \exp(-im\gamma), \quad (11)$$

where each matrix $d^{\ell}(\beta)$ is related to the group structure of the rotations, and can be computed by recurrence relations. As we will see in the next section, factorisation make it possible for the rotation function to be computed as a fourier transform, therefore opening the way to fast computation with the fast fourier transform.

Thank to (11), spherical harmonic $Y_{\ell}^m(\theta', \phi')$ can be re-written as

$$Y_{\ell}^m(\theta', \phi') = \sum_{m'=-\ell}^{\ell} \exp(-im'\alpha) d_{m' m}^{\ell}(\beta) \exp(-im\gamma) Y_{\ell}^{m'}(\theta, \phi)$$

Thus, the rotated patterson $Q(\Omega^{-1}\mathbf{r})$ will be expressed as,

$$Q(\Omega^{-1}\mathbf{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} b_{\ell m}(r) \sum_{m'=-\ell}^{\ell} \exp(-im'\alpha) d_{m' m}^{\ell}(\beta) Y_{\ell}^{m'}(\theta, \phi) \exp(-im\gamma)$$

4 Computing the rotation function with a fast fourier transform

The two patterns needed to compute the rotation function had their expression turned into spherical coordinates in the last two sections. We can now proceed to evaluate the integral defining this function:

$$\begin{aligned} \mathcal{R}(\alpha, \beta, \gamma) \equiv \int_S P(\mathbf{r})Q(\Omega^{-1}\mathbf{r})d\mathbf{r} = \\ \int_S \left\{ \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} a_{\ell m}(r)Y_{\ell}^m(\theta, \phi) \right\} \left\{ \sum_{\ell'=0}^{\infty} \sum_{m'=-\ell'}^{\ell'} b_{\ell' m'}(r) \right. \\ \left. \sum_{m''=-\ell'}^{\ell'} \exp(-im''\alpha) d_{m'' m'}^{\ell'}(\beta) Y_{\ell'}^{m''}(\theta, \phi) \exp(-im'\gamma) \right\} d\mathbf{r} = \end{aligned}$$

The integration volume is a sphere centred at the origin, say of radius R ; therefore the integration will be carried out from 0 to R for the variable r , from 0 to π for the variable θ , and from 0 to 2π for the variable ϕ . Also, the volume element is $d\mathbf{r} = r^2 \sin\theta d\theta d\phi$:

$$\begin{aligned} \mathcal{R}(\alpha, \beta, \gamma) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{\ell'=0}^{\infty} \sum_{m'=-\ell'}^{\ell'} \left\{ \int_0^R a_{\ell m}(r)b_{\ell' m'}(r)r^2 dr \right\} \\ \sum_{m''=-\ell'}^{\ell'} \exp(-im''\alpha) d_{m'' m'}^{\ell'}(\beta) \exp(-im'\gamma) \left\{ \int_0^{\pi} \int_0^{2\pi} Y_{\ell}^m(\theta, \phi) Y_{\ell'}^{m''}(\theta, \phi) \sin\theta d\theta d\phi \right\} \end{aligned}$$

Due to (2) the argument of last braces in the previous expression is equal to $\delta_{\ell\ell'}\delta_{mm''}$. So we have,

$$\mathcal{R}(\alpha, \beta, \gamma) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \sum_{m'=-\ell}^{\ell} \left\{ \int_0^R a_{\ell m}(r)b_{\ell m'}(r)r^2 dr \right\} \exp(-im\alpha) d_{mm'}^{\ell}(\beta) \exp(-im'\gamma)$$

or, if we indicate the integral on r as $c_{\ell mm'}$ and perform summation over ℓ first,

$$\mathcal{R}(\alpha, \beta, \gamma) = \sum_{m=-\ell}^{\ell} \sum_{m'=-\ell}^{\ell} \left\{ \sum_{\ell=0}^{\infty} c_{\ell mm'} d_{mm'}^{\ell}(\beta) \right\} \exp \left[-2\pi i \left(m \frac{\alpha}{2\pi} + m' \frac{\gamma}{2\pi} \right) \right] \quad (12)$$

We can now see very clearly from the above expression that $\mathcal{R}(\alpha, \beta, \gamma)$ is a fourier series, whose coefficients are given by the expression within braces.

We can now outline the major steps to compute a rotation function [1]:

1. the largest ℓ to be used, ℓ_{max} , is chosen;
2. the angular interval for β is sampled at n_{β} points. For each value of β , a summation $\sum_{\ell=0}^{\ell_{max}} c_{\ell mm'} d_{mm'}^{\ell}(\beta)$ is carried out (see next section for details). Basically, one matrix of size $(2\ell_{max} + 1) \times ((2\ell_{max} + 1))$ needs to be stored for each value of β ;
3. once all summations at previous point have been carried out and stored, we can evaluate the rotation function in sections of β as fast fourier transforms, given the fourier series at (12).

5 How data enter the game

In the previous section we have defined $c_{\ell mm'}$ as an integral over the radial interval, but we have not shown how this integral is calculated. The integral depends on $a_{\ell m}(r)$ and $b_{\ell m}(r)$ which, in turn, depend on experimental and calculated data (see (8) and (9)). Let us look a bit closer to the actual expression for this integral:

$$c_{\ell mm'} \equiv \int_0^R a_{\ell m}(r) b_{\ell m'}(r) r^2 dr$$

Replacing $a_{\ell m}(r)$ with formula (8) and $b_{\ell m'}(r)$ with formula (9),

$$c_{\ell mm'} = \frac{16\pi^2(-1)^\ell}{V} \sum_{\mathbf{s}} \sum_{\mathbf{s}'} |F(\mathbf{s})|^2 |G(\mathbf{s}')|^2 Y_\ell^{m*}(\theta_s, \phi_s) Y_\ell^{m'*}(\theta_{s'}, \phi_{s'}) \int_0^R j_\ell(2\pi s r) j_\ell(2\pi s' r) r^2 dr$$

or, with a change of variable,

$$c_{\ell mm'} = \frac{16\pi^2 R^3(-1)^\ell}{V} \sum_{\mathbf{s}} \sum_{\mathbf{s}'} |F(\mathbf{s})|^2 |G(\mathbf{s}')|^2 Y_\ell^{m*}(\theta_s, \phi_s) Y_\ell^{m'*}(\theta_{s'}, \phi_{s'}) \int_0^1 j_\ell(2\pi s R x) j_\ell(2\pi s' R x) x^2 dx$$

From the previous expression it is clear that the calculation is reduced to the evaluation of the following integral:

$$T_\ell(s, s') \equiv \int_0^1 j_\ell(2\pi s R x) j_\ell(2\pi s' R x) x^2 dx \quad (13)$$

Amazingly, the integral can be calculated analytically. The result is [5]:

$$T_\ell(s, s') = \begin{cases} [s j_{\ell-1}(2\pi R s) j_\ell(2\pi R s') - s' j_{\ell-1}(2\pi R s') j_\ell(2\pi R s)] / [2\pi R (s^2 - s'^2)] & \text{if } s \neq s' \\ 0.5 [j_\ell^2(2\pi R s) - j_{\ell-1}(2\pi R s) j_{\ell+1}(2\pi R s)] & \text{if } s = s' \end{cases} \quad (14)$$

Given that usually the number of reflections collected is quite high, the number of $T_\ell(s, s')$ to be computed is very high, and the number of times formula (14) has to be applied is very large. So, although $T_\ell(s, s')$ can be computed analytically, for the applications is better to calculate the integral defining $c_{\ell mm'}$ in a different way, either expanding each spherical Bessel function with a truncated fourier-bessel series, or with other numerical techniques (for details see [4]).

Appendices

A Legendre Polynomials and Associated Legendre Functions

A complete, orthogonal set of functions defined in the closed interval $-1 \leq x \leq 1$ is given by a family of polynomials called *Legendre polynomials*, and indicated as $P_n(x)$. They originate as finite solution of the well-known Legendre's equation, and can be generated using several series, integral and recurrence formulas. In this appendix we will define them through the so called *Rodrigues' formula*:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n \quad , \quad n = 0, 1, 2, 3, \dots \quad (15)$$

For example, the first four Legendre polynomials can be computed from (15) using $n = 0, 1, 2, 3$, thus giving,

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= (1/2)(3x^2 - 1) \\ P_3(x) &= (1/2)(5x^3 - 3x) \end{aligned}$$

In many applications $x \equiv \cos \theta$, so that $-1 \leq x \leq 1$. In this article, for instance, θ represents one of the spherical coordinates. The *associated Legendre functions*, $P_\ell^m(x)$, are themselves defined in the closed interval $[-1, 1]$. They can be computed starting from Legendre polynomials through the following formula:

$$\begin{aligned} P_\ell^m(x) &\equiv (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x) \\ P_\ell^{-m}(x) &\equiv (-1)^m \frac{(\ell - m)!}{(\ell + m)!} P_\ell^m(x) \end{aligned} \quad 0 \leq m \leq \ell \quad (16)$$

In the above relations it is important to highlight that, once ℓ has been chosen, m has to be smaller or equal to ℓ . Therefore, a Legendre polynomial of degree ℓ gives rise to $2\ell + 1$ associated Legendre functions. For instance, starting from Legendre polynomial $P_2(x)$ we can build five associated Legendre functions:

$$\begin{aligned} P_2^2(x) &= 3(1 - x^2) \\ P_2^1(x) &= 3x\sqrt{1 - x^2} \\ P_2^0(x) &= (1/2)(3x^2 - 1) \\ P_2^{-1}(x) &= (-1/2)x\sqrt{1 - x^2} \\ P_2^{-2}(x) &= (1/8)(1 - x^2) \end{aligned}$$

The associated Legendre function obey the following orthogonality relations:

$$\int_{-1}^1 P_\ell^m(x) P_{\ell'}^m(x) dx = \frac{2}{2\ell + 1} \frac{(\ell + m)!}{(\ell - m)!} \delta_{\ell\ell'} \quad (17)$$

In the above integral m is the same for both Legendre functions, only the lower indices are different. A relation analogous to (17) exists when the lower indices are the same and the upper ones different, but it is rarely used. If, rather than using the variable x we use θ in $x = \cos \theta$, the orthogonality relations has to be re-written as follows,

$$\int_0^\pi P_\ell^m(\cos \theta) P_{\ell'}^m(\cos \theta) \sin \theta d\theta = \frac{2}{2\ell + 1} \frac{(\ell + m)!}{(\ell - m)!} \delta_{\ell\ell'} \quad (18)$$

B Spherical Harmonics

In many physical problems the angular part of a given equation can be isolated, thus giving origin to a function depending only on angular variables, typically θ and ϕ ($0 \leq \theta \leq \pi$, $0 \leq \phi < 2\pi$). Given the ubiquity of functions depending on angular space variables in all subfields of physics, it is important to have an orthogonal set with which any of these functions can be expanded as a series in an angular range. As θ and ϕ vary on the surface of a sphere (centred at the origin and of arbitrary radius), we will be talking about series expansion “on the sphere”. The orthogonal functions normally used for the expansion on the sphere are called *spherical harmonics*. They are symbolically indicated as $Y_l^m(\theta, \phi)$ and defined as follows,

$$Y_l^m(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) \exp(im\phi), \quad \begin{matrix} l = 0, 1, 2, 3, \dots \\ -l \leq m \leq l \end{matrix} \quad (19)$$

Sometimes a sign (or phase) factor, $(-1)^m$ is prepended to definition (19). This is known as *Condon-Shortley phase*, and it is a convenient choice for applications related to quantum mechanics.

A simple relation exists between $Y_l^m(\theta, \phi)$ and $Y_l^{-m}(\theta, \phi)$. It is quite straightforward to derive it. We start from definition (19),

$$Y_l^{-m}(\theta, \phi) = \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}} P_l^{-m}(\cos \theta) \exp(-im\phi),$$

then replace P_l^{-m} with second equation in (16),

$$\begin{aligned} Y_l^{-m}(\theta, \phi) &= \sqrt{\frac{2l+1}{4\pi} \frac{(l+m)!}{(l-m)!}} (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\cos \theta) \exp(-im\phi) \\ &\quad \downarrow \\ Y_l^{-m}(\theta, \phi) &= (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos \theta) \exp(-im\phi) \equiv (-1)^m Y_l^{m*}(\theta, \phi) \end{aligned}$$

We have, thus, proved that,

$$Y_l^{-m}(\theta, \phi) = (-1)^m Y_l^{m*}(\theta, \phi) \quad (20)$$

Let us write, for example, the five spherical harmonics with $\ell = 2$. First let us calculate Y_2^0 , Y_2^1 , Y_2^2 using formula (19); then it is easier to compute Y_2^{-1} and Y_2^{-2} through relation (20).

$$\begin{aligned} Y_2^0(\theta, \phi) &= \sqrt{\frac{5}{4\pi}} P_2^0(\cos \theta) = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1) \\ Y_2^1(\theta, \phi) &= \sqrt{\frac{5}{4\pi} \frac{1}{3!}} P_2^1(\cos \theta) \exp(i\phi) = \sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta \exp(i\phi) \\ Y_2^2(\theta, \phi) &= \sqrt{\frac{5}{4\pi} \frac{1}{4!}} P_2^2(\cos \theta) \exp(2i\phi) = \sqrt{\frac{15}{32\pi}} \sin^2 \theta \exp(2i\phi) \end{aligned}$$

Now Y_2^{-1} and Y_2^{-2} are readily computed as,

$$\begin{aligned} Y_2^{-1}(\theta, \phi) &= -Y_2^{1*}(\theta, \phi) = -\sqrt{\frac{15}{8\pi}} \cos \theta \sin \theta \exp(-i\phi) \\ Y_2^{-2}(\theta, \phi) &= Y_2^{2*}(\theta, \phi) = \sqrt{\frac{15}{32\pi}} \sin^2 \theta \exp(-2i\phi) \end{aligned}$$

We have said that any function of θ and ϕ (behaving sufficiently well), $f(\theta, \phi)$, can be expanded in spherical harmonics series:

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l a_{lm} Y_l^m(\theta, \phi) \quad (21)$$

A double summation is needed here because each spherical harmonic is identified by two indices. We know how to compute coefficients a_{lm} only if the spherical harmonics form an orthogonal set. The orthogonality of the spherical harmonics can, quite appropriately, be defined as,

$$\int_0^{\pi} \int_0^{2\pi} Y_l^{m*}(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \sin \theta d\theta d\phi = \delta_{ll'} \delta_{mm'} \quad (22)$$

It just needs to be proved it is true. Using definition (19) we have,

$$\begin{aligned} & \int_0^{\pi} \int_0^{2\pi} Y_l^{m*}(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \sin \theta d\theta d\phi = \\ & \sqrt{\frac{(2l+1)(2l'+1)}{16\pi^2} \frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}} \int_0^{\pi} \int_0^{2\pi} P_l^m(\cos \theta) P_{l'}^{m'}(\cos \theta) \exp[i(m'-m)] \sin \theta d\theta d\phi = \\ & \sqrt{\frac{(2l+1)(2l'+1)}{4} \frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}} \int_0^{\pi} P_l^m(\cos \theta) P_{l'}^{m'}(\cos \theta) \sin \theta d\theta \left\{ \frac{1}{2\pi} \int_0^{2\pi} \exp[i(m'-m)] d\phi \right\} \end{aligned}$$

The integral in braces is a well-known integral. It is always zero, unless $m' = m$, in which case it is 1. Therefore,

$$\begin{aligned} & \int_0^{\pi} \int_0^{2\pi} Y_l^{m*}(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \sin \theta d\theta d\phi = \\ & \sqrt{\frac{(2l+1)(2l'+1)}{4} \frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!}} \int_0^{\pi} P_l^m(\cos \theta) P_{l'}^m(\cos \theta) \sin \theta d\theta \delta_{mm'} \end{aligned}$$

The integral on the right-hand side can be computed with formula (18). We obtain, thus,

$$\begin{aligned} & \int_0^{\pi} \int_0^{2\pi} Y_l^{m*}(\theta, \phi) Y_{l'}^{m'}(\theta, \phi) \sin \theta d\theta d\phi = \\ & \sqrt{\frac{(2l+1)(2l'+1)}{4} \frac{(l-m)!(l'-m')!}{(l+m)!(l'+m')!} \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!}} \delta_{ll'} \delta_{mm'} = \delta_{ll'} \delta_{mm'}, \end{aligned}$$

that is, result (22). Through property (22) it is possible, quite straightforwardly, to find coefficients a_{lm} in the expansion (21). They are given by the following formula,

$$a_{lm} = \int_0^{\pi} \int_0^{2\pi} f(\theta, \phi) Y_l^{m*}(\theta, \phi) \sin \theta d\theta d\phi \quad (23)$$

C Spherical Bessel Functions of the First Kind

Bessel functions of the first kind are particular solutions of Bessel's equation, finite at $x = 0$. They are normally indicated as $J_m(x)$ and the parameter m can take any positive or null real value. Bessel functions can only be expressed as infinite, but converging, summations of powers of x . When m is equal to a semi-integer, though, closed analytic forms are available. For instance,

$$\begin{aligned} J_{1/2}(x) &= \sqrt{2/(\pi x)} \sin x \\ J_{3/2}(x) &= \sqrt{2/(\pi x)} (\sin x/x - \cos x) \\ J_{5/2}(x) &= \sqrt{2/(\pi x)} [(3/x^2 - 1) \sin x - (3/x) \cos x] \\ &\dots \end{aligned}$$

The *spherical Bessel functions* are defined starting from Bessel functions with semi-integer m , in the following way:

$$j_\ell(x) \equiv \sqrt{\frac{\pi}{2x}} J_{\ell+1/2}(x) \quad , \quad \ell = 0, 1, 2, 3, \dots \quad (24)$$

Thus, the first three spherical Bessel functions are:

$$\begin{aligned} j_0(x) &= \sin x/x \\ j_1(x) &= \sin x/x^2 - \cos x/x \\ j_2(x) &= (3/x^3 - 1/x) \sin x - (3/x^2) \cos x \\ &\dots \end{aligned}$$

These functions have a typically oscillatory character (see plots in Figure 2), but their zeroes occurs, differently from the zeroes of the trigonometric functions, at irregular intervals, and are found through tables or numerical methods.

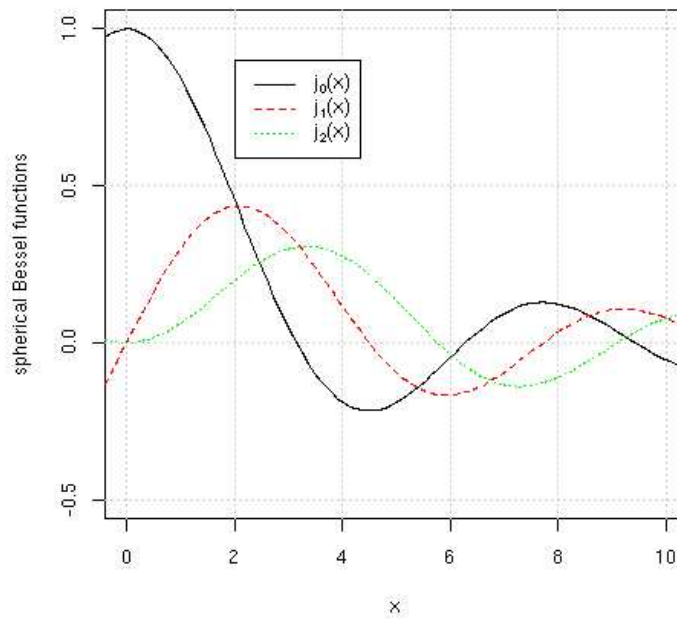


Figure 2: Plots of the first three spherical Bessel functions.

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