YALE UNIVERSITY

Department of Physics

SO(3) Invariants of Spherical Functions

Student:
Joseph Balsells

Supervisor:
Prof. George Fleming

Abstract

Invariant parts of spherical functions are discussed. The SO(3) invariants of both 1-point and 2-point spherical functions are exhibited explicitly. Some direction is provided for generalizing these techniques to 3-point functions through the Racah coefficients. The role of parity is discussed. The cosmic microwave background is used as an example of the methods developed.

Introduction

Physical laws are defined by the symmetries they preserve. Symmetry gives, by definition, a number of equivalent states for a system. However all systems which come into existence must break their symmetry by choosing one of the allowed states. This is a basic ontological consequence – while the physical laws themselves obey symmetries, the initial conditions often do not. This poses a problem for experimental physics where we do not know the laws ahead of time and it is only through observation that we gain an understanding of them. When we have only one or a few chances to view such a system we have to be careful about the conclusions that we draw. How do we separate circumstance from physical law?

Take for example a pencil standing on its tip. It is equally likely to fall in any direction but it can only choose one. If we only observe the pencil falling once we might make the assumption that some law of the system caused the pencil to fall in the direction it did. If however we had an ensemble of many pencils and watched all of them fall then the symmetry would become apparent. On the other hand, if we know the correct symmetry, then we would not need the ensemble. Knowing the full symmetry allows us to make statements about a system which are independent of any particular realization. By knowing what pieces of a system are invariant under the symmetry we make conjectures on the laws of the system based only on those invariants. Hence an important question in physics asks what the invariants are of a given symmetry. In this paper we will be concerned with finding invariants of rotational symmetry for functions defined on a sphere. Much of this theory has been worked out in the last century by Eugene Wigner (see references).

The outline for this paper is as follows. First we discuss the representation theory of the rotation group SO(3). We then apply these results to derive two simple SO(3) invariants of an arbitrary function on a sphere, namely its average and its angular power spectrum. We provide some comments on how to extend these results to finding more invariants. We also discuss extending the symmetry to the full orthogonal group O(3). This naturally differentiates invariants of scalar and pseudoscalar functions. Although the results we present are quite general, an important motivation for their study is provided from the astrophysics community and the cosmic microwave background radiation (CMB). At the end we provide a brief discussion of CMB physics.

Representation Theory of SO(3)

Every rotation is a symmetry by preserving the standard inner product on $\mathbb{R}^3$. That is, if we define the inner product for any two vectors, $x, y \in \mathbb{R}^3$ as

$$\langle x, y\rangle \equiv x^T y \equiv x^1 y^1 + x^2 y^2 + x^3 y^3$$

then we require the rotation R to satisfy

$$\langle Rx, Ry\rangle = \langle x, y\rangle$$

Writing this out we find

$$\langle Rx, Ry\rangle = (Rx)^T(Ry) = x^T(R^TR)y$$

giving the condition $R^TR = I$. Such a transformation on $\mathbb{R}^3$ is called *orthogonal*. The set of orthogonal transformations on $\mathbb{R}^3$ defines the matrix Lie group O(3). Taking determinants we find that R must also satisfy $\det(R) = \pm 1$. The negative determinant matrices correspond to parity inversions of the space. The positive determinant matrices form a subgroup of O(3) called the *special orthogonal group* denoted SO(3).

To say that SO(3) is a Lie group means that the group elements are related by several continuous parameters. The two relations $R^TR = I$ and $\det(R) = 1$ tell us that SO(3) has three parameters. In the case of SO(3) there are three common parameterizations. Before we discuss these parameterizations it will be useful to state the associated Lie Algebra. The three generators are called J_x, J_y, and J_z and they satisfy the commutation relations $[J_i, J_j] = i\epsilon_{ijk}J_k$. It is easy to check that a rotation by α about the x-axis is given by $e^{-i\alpha J_x}$. From these commutation relations we deduce that SO(3) has representations labeled by an integer l of dimension $2l + 1$. We may refer to an abstract basis for these representations using kets labeled as $|lm\rangle$ or more concretely using spherical harmonics defined as

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

where P_l^m are the associated Legendre polynomials and the normalization ensures

$$\iint Y_l^{m*}Y_{l'}^{m'}\,d\Omega = \delta_{ll'}\delta^{mm'}$$

These functions are complete and any function f on a sphere can be expanded in a uniformly convergent series of spherical harmonics.

$$f(\theta, \phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{m=1} a_{lm}Y_l^m(\theta, \phi)$$

The coefficients are computed in the regular way as the projection of the basis vectors onto the function

$$a_{lm} = \left\langle Y_l^m \,\middle|\, f(\theta, \phi)\right\rangle = \int d\phi \int \sin\theta\; d\theta\; Y_l^m(\theta, \phi)^* f(\theta, \phi)$$

Since the spherical harmonics for given l define a representation of SO(3) they behave nicely under rotations, transforming into linear combinations of themselves

$$Y_l^m(R\Omega) = \sum_{m'} D^l_{m'm}(R) Y_l^{m'}(\Omega)$$

Where we the expansion coefficients $D^l_{m'm}(R)$ depends on the rotation, R. The $D^l_{m'm}(R)$ are the Wigner matrices. The explicit form of the Wigner matrices depends on the parameterization of the group chosen and we now discuss the three common parameterizations of the group.

In the first an arbitrary rotation is achieved by successive rotations about three mutually orthogonal *fixed* axes. This is perhaps the simplest parameterization to think of but not necessarily the most useful. An alternative is to define rotation with respect to three comoving axes. In practice means choosing a first axis to rotate around, usually z, and to rotate by an angle α. Then one would rotate around one of the *new* x- or y-axes. We will assume the second rotation is one by angle β about the new y-axis. The final rotation is then about another one of the new axes. We assume this to be the new z-axis and by angle γ. The standard notation for these conventions is to say that we have chosen the $Z_\alpha - Y_\beta - Z_\gamma$ parameterization. The angles α, β, γ are called Euler angles. The final common parameterization is the axis-angle representation given by specifying an axis to rotate about and the angle by which to rotate.

Using the Euler angle parameterization an arbitrary rotation can be written

$$R(\alpha, \beta, \gamma) = e^{-i\alpha J_z} e^{-i\beta J_z} e^{-i\gamma J_z}$$

And the Wigner matrices take the more explicit form

$$D^l_{m'm}(R(\alpha, \beta, \gamma)) = Y_l^{m'*} R(\alpha, \beta, \gamma) Y_l^m = e^{-im'\alpha} d^l_{m'm}(\beta) e^{-im\gamma}$$

where $d^l_{m'm}$ is Wigner's small d-matrix. This has an explicit form in terms of β but it is rather complicated.

The 1-point function

We start by examining the simplest case of a scalar function of one point on the sphere. Call this function $f = f(\Omega)$. We wish to determine the spherically invariant piece of this function, that is, the piece $\tilde{f}$ which satisfies $\tilde{f}(R\Omega) = \tilde{f}(\Omega)$. It is clear that this invariant part of f can only have trivial angular dependence if it is to remain invariant under arbitrary rotations – the only function which is unaffected by rotation is the constant function $f(\Omega) = f_o$. Intuitively, for an an arbitrary function f which is not constant over the sphere we expect this invariant part to be its average over the sphere. No matter where you look you expect the average value to be the same. We may extract this invariant part in two equivalent ways. The most explicit is to average the function over all rotations. That is, define the invariant part as

$$\tilde{f}(\Omega) \equiv \int_{\mathrm{SO}(3)} f(R\Omega) dR$$

Then we can prove that this is in fact invariant under arbitrary rotation by appealing to the rearrangement theorem. For a finite group $G = \{e, a, b, \ldots, n\}$ the rearrangement theorem states

$$aG = \{a, a^2, ab, \ldots, an\} = G$$

That is, multiplying every element of the group by some fixed element merely permutes the elements without removing one or adding something new. We may state the theorem equivalently given a function which is summed over all group elements as

$$\sum_g f(g) = \sum_g f(g'g)$$

All terms appear on both sides, only perhaps in a different order. For finite groups the proof of this theorem is trivial. The statement of this theorem carries over in a natural way to compact Lie groups when we replace the sum by an integral and may be stated as

$$\int f(R) dR = \int f(R'R) dR$$

Because this is a compact group the integral should converge. The only thing we need to be careful about is the integration measure. The form of the measure depends on the parameterization of the group as $dR = \mu(R) da_1 da_2 \ldots da_r$ where $\mu(R)$ is the group density at R and the differentials are the parameter differentials. The proof of the rearrangement theorem for compact groups relies upon this integration measure being constant across the group. Notationally we write $\mu(R) = \mu(I)$. Since this theorem holds for the group SO(3) we can show that $\tilde{f}$ defined above really is the invariant part of the 1-point function:

$$\tilde{f}(R\Omega) = \int_{\mathrm{SO}(3)} f(RR'\Omega) dR' = \tilde{f}(\Omega)$$

Indeed $\tilde{f}$, whatever it is, is invariant under arbitrary rotation. At this point it would be possible to give a more explicit form for $\tilde{f}$ in terms of this integral by substituting the spherical harmonic decomposition and the Euler angle parameterization. This is rather involved. Instead we know almost by definition that the invariant part must be that given by the trivial representation, that is the Y_0^0 term of its spherical harmonic decomposition. Also the natural constant function we can define for an arbitrary function is its average. We can show that the Y_0^0 term in fact does correspond to the average of the function over the sphere

$$
\begin{aligned}
\big\langle f(\theta,\phi)\big\rangle_{\text{sphere}} &= \frac{1}{4\pi}\iint f(\theta,\phi)\sin\theta\; d\theta d\phi \\
&= \frac{1}{4\pi}\iint \Big(\sum_{l,m} a_{lm}Y_l^m\Big)\sin\theta\; d\theta d\phi \\
&= \frac{1}{4\pi}\sum_{l,m} a_{lm}\iint Y_l^m \sin\theta\; d\theta d\phi \\
&= \frac{1}{4\pi}\sum_{l,m} a_{lm}\int_0^{2\pi} d\phi\; e^{im\phi}\int_0^{\pi}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{l+m)!}}P_l^m(\cos\theta)\sin\theta\; d\theta \\
&= \frac{1}{4\pi}\sum_{l,m} a_{lm}2\pi\delta_{m,0}\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{l+m)!}}\int_{-1}^{1} P_l^m(x)\; dx \\
&= \frac{1}{2}\sum_{l} a_{l0}\sqrt{\frac{2l+1}{4\pi}}\int_{-1}^{1} P_l^m(x)\; dx \\
&= a_{00}\frac{1}{\sqrt{4\pi}} \\
&= a_{00}Y_0^0
\end{aligned}
$$

Which confirms that Y_0^0 gives the average of f in the sense that it is the unique quality of f at a single point which remains unchanged by an arbitrary rotation. Our story does not end here. We can build more complicated rotation invariants. To do this we must look at more complicated objects.

Invariants of the scalar 2-point function

Consider a function of two points on the sphere, $g = g(\Omega_1,\Omega_2)$. This could take many forms. For example,

$$
\begin{aligned}
g(\Omega_1,\Omega_2) &= f_1(\Omega_1) \pm f_2(\Omega_2) \\
g(\Omega_1,\Omega_2) &= f_1(\Omega_1) f_2(\Omega_2)
\end{aligned}
$$

In fact, to be totally general we can decompose f_1 and f_2 into spherical harmonics and determine the most general function of two points

$$g(\Omega_1, \Omega_2) = \sum_{l_1} \sum_{l_2} \sum_{m_1} \sum_{m_2} b_{l_1 l_2}^{m_1 m_2} Y_{l_1}^{m_1}(\Omega_1) Y_{l_2}^{m_2}(\Omega_2)$$

Clearly both of the cases above are subsumed by writing g in this way. We wish to extend the result above to determine the rotationally invariant part of a function of two points. Schematically we want $\tilde{g}(R\Omega_1, R\Omega_2) = \tilde{g}(\Omega_1, \Omega_2)$. This part is determined explicitly by the rearrangement theorem by defining

$$\tilde{g}(\Omega_1, \Omega_2) = \int_{\mathrm{SO(3)}} g(R\Omega_1, R\Omega_2) dR$$

The form of $\tilde{g}$ could again be determine explicitly by substituting the double spherical harmonic expansion into this and utilizing the Euler angle parameterization. However this is also rather involved. We can get around this again by guessing at the correct form and showing it to be correct Define

$$A = \sum_{m=-1}^{l} Y_l^m(\Omega_1)^* Y_l^m(\Omega_2)$$

Under rotation,

$$\begin{aligned}
RA &= \sum_m \left(\sum_\mu D_{\mu m}^l(R) Y_l^\mu(\Omega_1) \right)^* \left(\sum_\nu D_{\nu m}^l(R) Y_l^\nu(\Omega_2) \right) \\
&= \sum_{\mu\nu} \left(\sum_m D_{\mu m}^l(R)^* D_{\nu m}^l(R) \right) Y_l^\mu(\Omega_1)^* Y_l^\nu(\Omega_2) \\
&= \sum_{\mu\nu} \left(\sum_m \left[D^l(R)^{-1} \right]_{m\mu} \left[D^l(R) \right]_{\nu m} \right) Y_l^\mu(\Omega_1)^* Y_l^\nu(\Omega_2) \\
&= \sum_{\mu\nu} \delta_{\mu\nu} Y_l^\mu(\Omega_1)^* Y_l^\nu(\Omega_2) \\
&= \sum_\mu Y_l^\mu(\Omega_1)^* Y_l^\mu(\Omega_2) = A
\end{aligned}$$

That is, A is a rotational invariant. This proof relied crucially on the unitarity of the Wigner matrices. Given that A is rotationally invariant we are free to rotate it into any position that is convenient. So we send $\Omega_1 = (\theta_1, \phi_1)$ and $\Omega_2 = (\theta_2, \phi_2)$ to the special points $\Omega_1' = (0, \phi)$ and $\Omega_2' = (\chi, 0)$. The first is the north pole and the second is along the prime meridian. Note that χ is defined as the angle between Ω_1 and Ω_2. Performing this substitution allows us to replace the spherical harmonics with their simplified forms.

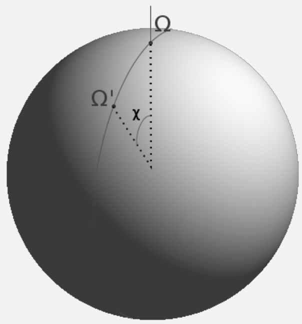


Figure 1: The simplest orientation for a two-point function is to send one point to the north pole and the other to lie along the prime meridean.

$$Y_l^m(\Omega_1') = \sqrt{\frac{2l+1}{4\pi}}\delta_{m0}$$

The δ_{m0} reduces the summation defining A to only the $m = 0$ terms which allows us to simplify the other harmonic term

$$Y_l^0(\chi, \phi_2) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\chi)$$

Hence we obtain

$$A = \frac{2l+1}{4\pi} P_l(\cos\chi)$$

Combining this with our defining equation for A we obtain the result of the Spherical Harmonic Addition Theorem.

$$P_l(\cos\chi) = \frac{4\pi}{2l+1}\sum_m Y_l^{m*}(\Omega_1)Y_l^m(\Omega_2)$$

If we rearrange this slightly, multiply by $|a_{lm}|^2$ and sum over l we obtain

$$\sum_l \sum_m \left[a_{lm}Y_l^m(\Omega_1)\right]^* a_{lm}Y_l^m(\Omega_2) = \sum_l \frac{2l+1}{4\pi}|a_{lm}|^2 P_l(\cos\chi)$$

Which defines the 2-point correlation function

$$\langle \Omega_1, \Omega_2 \rangle = \sum_l \frac{2l+1}{4\pi} C_l P_l(\cos\chi)$$

Where the $C_l = \frac{1}{2l+1}\sum_m |a_{lm}|^2$ define the angular power spectrum. This expansion in Legendre polynomials is rotationally invariant. For the two-point function we have $\tilde{g}(\Omega_1, \Omega_2) = \langle \Omega_1, \Omega_2 \rangle$. Intuitively what this tells us is that for an arbitrary function which arises from spherically symmetric processes what we care about is only the strength of fluctuations at a given scale.

What we have just done is made more easily accessible when we view the two point function g in terms of angular momentum. Instead of expressing g as a quadruple sum over l_1, l_2, m_1, m_2, the theory of angular momentum developed in quantum mechanics allows us to change basis and think of g as the sum of components of definite total angular momentum L. We may define rank-two spherical tensors (bipolar spherical harmonics) as bilinear products of spherical harmonics with different arguments coupled to total angular momentum. This definition relies upon the well-known Clebsch-Gordan series

$$B_{LM}^{l_1 l_2}(\Omega_1, \Omega_2) = \sum_m C(l_1, l_2, L; m, M-m, M)\, Y_{l_1}^m(\Omega_1) Y_{l_2}^m(\Omega_2)$$

The quantities $B_{LM}^{l_1 l_2}$ encode interactions (correlations) between different spatial scales, $a_{l_1 m_1}, a_{l_2 m_2}$. Phrased in this basis g becomes a sum over these states of definite total angular momentum

$$g(\Omega_1, \Omega_2) = \sum_{L=0}^{\infty} \sum_{M=-L}^{L} b_{LM} B_{LM}(\Omega_1, \Omega_2)$$

Now it is manifestly evident that the rotationally invariant part of g is given by B_{00} – the trivial representation of SO(3). We see from the definition that B_{00} must correspond to the result of the addition theorem and the angular power spectrum. But what then do the higher moments of the B_{LM} correspond to? Many in the astrophysics community view these as the tool to understanding departures from isotropy in the cosmic microwave background. But in an entirely analogous way to how we formed the angular power spectrum out of the spherical harmonic decomposition in the addition theorem, we should be able to form a rank-two power spectrum out of this bipolar harmonic decomposition. In 1968 Yasuo Munakata gave precisely this generalization of the spherical harmonic addition theorem to sums of the bipolar spherical harmonics. The resulting polynomial which corresponds to the Legendre polynomial is a finite series of the Gegenbauer polynomials.

Now we recognize that we can continue building up more and more complicated functions to describe more and more SO(3) invariants of any function. For example we can consider coupling three angular momenta l_1, l_2, l_3 to give a resultant L. The first difficulty with this procedure is that there are two ways to complete this coupling. We may first couple l_1 to l_2 and then couple their resultant to l_3. Alternatively we may first couple l_2 and l_3 and then couple their resultant to l_1. These two routes are related by a unitary transformation, but are not in general exactly equivalent. The elements of this unitary matrix are the Racah coefficients whose symmetry properties are related to those of the Clebsch-Gordan coefficients by the 3-j and 6-j symbols.

This scheme can be extended in the obvious, though computational intensive way to arbitrary combinations of angular momentum giving more information

Parity

We conclude the main development with a short note on the role of parity. We recognize that the arbitrary function $f(\Omega)$ does not have a well-defined parity by the parity property of the spherical harmonics: Under parity inversion $(\theta, \phi) \mapsto (\pi - \theta, \phi \pm \pi)$ and $Y_l^m(\Omega) \mapsto (-1)^l Y_l^m(\Omega)$. Thus our decomposition of f breaks up into even and odd parity parts

$$Pf = \sum_l (-1)^l \sum_m a_{lm} Y_l^m(\Omega) = f_0 - f_1 + f_2 - f_3 + \dots$$

Using these symmetry properties we can define two functions

$$f_{\text{odd}} = \sum_{l \text{ odd}} \sum_m a_{lm} Y_l^m$$

$$f_{\text{even}} = \sum_{l \text{ even}} \sum_m a_{lm} Y_l^m$$

$Pf_{\text{even}} = f_{\text{even}}$	$Pf_{\text{odd}} = -f_{\text{odd}}$
(scalar 1-point function)	(pseudo-scalar 1-point function)

We notice immediately that pseudo-scalar functions do not have any 1-point SO(3) invariants! However both scalar functions and pseudoscalar functions exhibit the Legendre polynomial decomposition as two-point invariants. This question of parity should be pursued and understood at the level of the bipolar spherical harmonics and their invariants.

Cosmic Microwave Background

The cosmic microwave background is a low energy radiation field first predicted in the 1940s and detected in the 1960s. The radiation was created early in the history of the universe when matter and radiation decoupled. In the astrophysics community it is understood to be the cleanest and most direct information about the early universe. The temperature map (3) is characterized foremost by its isotropy. The standard deviation of the whole-sky map is only on the order of 100 milliKelvin. However detailed measurements indicate the presence of anisotropies. These anisotropies are recognized as stemming from two sources. Primary anisotropies refer to effects that occurred at the last scattering surface and before. Secondary anisotropy refers to effects which have affected the map since then including interactions of the radiation with hot gas or gravitational potentials. Both source of anisotropy provide useful information to astrophysicists. The primary anisotropies place constraints on inflation, the geometry of the universe, baryon density, and dark matter. The secondary anisotropies indirectly provide information of galaxy formation.

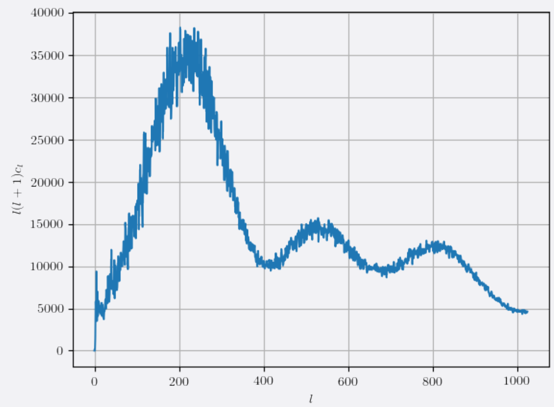
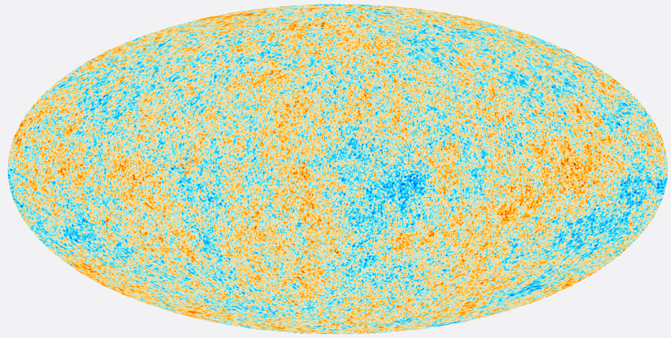


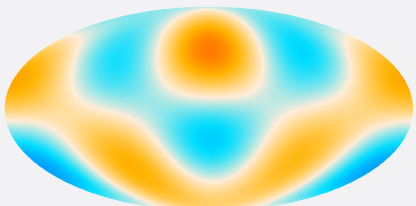
Figure 2: CMB angular power spectrum.

In studying the CMB, any information about these anisotropies has to survive an arbitrary rotation because the laws which created them are rotationally invariant. We can imagine an ensemble universes, each exactly like our own but each rotated arbitrarily. The ensemble average CMB contains the only information about the CMB physics independent of initial conditions.

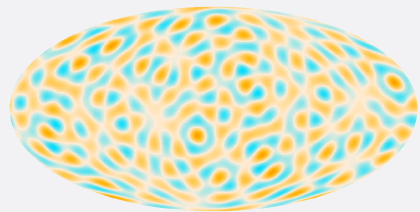
The 1-point invariant, the average, is well known to be about 2.7K. This places constraints on the age of the radiation. The more interesting results come from the angular power spectrum afforded as 2-point invariants.



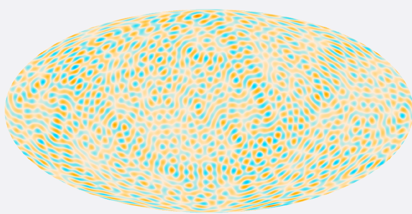
(a) Full CMB



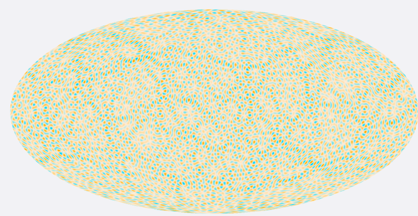
(b) l=3



(c) l = 20



(d) l=50



(e) l=100

Figure 3: The cosmic microwave background temperature map in Mollweide projection as measured by WMAP. Data retrieved from https://lambda.gsfc.nasa.gov/product. Subfigures show the CMB contribution from distinct angular momenta. All plots were generated by me.

References

Papers:

Coble, K., et al. 2003 *ApJ* 584, 585-592.
Hu, W., Dodelson, S., 2002 *ARA&A*, 40, 171.
Munakata, Y. 1968. *Commun. math. Phys.* 9, 18-37.

Textbooks:

Edmonds, A.R., *Angular Momentum in Quantum Mechanics*, Princeton University Press. 1957.
Jansen, L., Boone, M., *Theory of Finite Groups. Applications in Physics*. Elsevier. 1967.
Rose, M.E., *Elementary Theory of Angular Momentum*. John Wiley & Sons. New York. 1957.
Wigner, E. *Group Theory and its Application to the Quantum Mechanics of Atomic Spectra*. Trans. J.J. Griffin. Academic Press. 1959.

Presentations

Eriksen, H.K., An Introduction to the CMB Power Spectrum. http://folk.uio.no/hke/AST5220/v11/AST5220_2_2011.pdf. 2011.

Hivon, E., Galli, S., CMB Angular Power Spectra and Their Likelihoods in Theory and in (Planck) Practice. 2017.