Appendix 1

The irreducible representation matrices for the rotation group and the rotation functions $d^j_{\lambda\mu}(\theta)$

We present here some useful properties of the unitary matrices $\mathscr{D}^{(j)}_{m'm}(r)$, $j = 0, 1/2, 1, 3/2, \ldots, -j \le m, m' \le j$, which form an irreducible representation of the operation corresponding to an arbitrary rotation r. We also give a simple method for calculating them. Our conventions for describing r are explained in Section 1.1. We follow the notation of Jacob and Wick (1959). Detailed discussions of the rotation group can be found in the books of Rose (1957), whose notation is the same as ours, and of Edmonds (1957), whose notation differs from ours, as will be explained below.

The most general rotation, through Euler angles α, β, γ, is given in (1.2.17). The unitary operator $U(r)$ corresponding to this rotation can be expressed in terms of the angular momentum operators J_x, J_y, J_z, which are the generators of rotations. One has

$$U[r(\alpha, \beta, \gamma)] = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z}. \tag{A1.1}$$

It follows from (1.1.20) that

$$\mathscr{D}^{(j)}_{\lambda\mu}(\alpha, \beta, \gamma) = e^{-i\lambda\alpha} d^j_{\lambda\mu}(\beta) e^{-i\mu\gamma} \tag{A1.2}$$

where[1]

$$d^j_{\lambda\mu}(\beta) = \left\langle j\lambda | e^{-i\beta J_y} | j\mu \right\rangle. \tag{A1.3}$$

Note that for clarity we are here using λ, μ instead of m' and m respectively.

The d-functions enjoy several symmetry properties:

$$d^j_{\lambda\mu}(\beta) = d^j_{-\mu-\lambda}(\beta) = (-1)^{\lambda-\mu} d^j_{\mu\lambda}(\beta) \tag{A1.4}$$

[1] Note that the functions $\mathscr{D}^{(j)}_{\lambda\mu}(\alpha, \beta, \gamma)$ and $d^j_{\lambda\mu}(\beta)$ in Edmond's book correspond to our $\mathscr{D}^{(j)}_{\lambda\mu}(-\alpha, -\beta, -\gamma)$ and $d^j_{\lambda\mu}(-\beta)$ respectively.

https://doi.org/10.1017/9781009402040.015 Published online by Cambridge University Press

$$d^j_{\lambda\mu}(\beta) = (-1)^{j+\lambda} d^j_{\lambda,-\mu}(\pi - \beta) \tag{A1.5}$$

$$d^j_{\lambda\mu}(-\beta) = d^j_{\mu\lambda}(\beta). \tag{A1.6}$$

Procedures for the computation of the d-functions are described in Edmonds (1957) and in Jacob and Wick (1959). However, as we shall explain below, the disadvantage of these methods is that they produce expressions for the d-functions that do not show explicitly certain key features, for example that

$$d^j_{\lambda\mu}(\beta) = (\sin\beta/2)^{|\lambda-\mu|}(\cos\beta/2)^{|\lambda+\mu|} \times (\text{polynomial in } z = \cos\beta). \tag{A1.7}$$

The angular factors are of crucial importance for $\beta \to 0$ or π, as discussed in Chapter 4. We shall therefore modify the published methods so as to make explicit the structure (A1.7).

Our starting point is the relation given in Jacob and Wick (1959):

$$d^j_{\lambda,\mu\pm1}(\beta) = \frac{1}{\sqrt{(j\pm\mu+1)(j\mp\mu)}} \times \left(-\frac{\lambda}{\sin\beta} + \mu\cot\beta \mp \frac{d}{d\beta}\right) d^j_{\lambda,\mu}(\beta). \tag{A1.8}$$

Let us define

$$d^j_{\lambda,\mu}(\beta) \equiv (\sin\beta/2)^{|\lambda-\mu|}(\cos\beta/2)^{|\lambda+\mu|} \times \left[\frac{(j-\lambda)!(j-\mu)!}{(j+\lambda)!(j+\mu)!}\right]^{1/2} P^j_{\lambda,\mu}(\cos\beta) \tag{A1.9}$$

where $P^j_{\lambda,\mu}$ is a polynomial in $\cos\beta$. Then after some algebra (A1.8) can be written, for the case which will be of interest to us, as

$$\begin{aligned} d^j_{\lambda,\mu+1}(\beta) = {} & \tfrac{1}{4}(\sin\beta/2)^{|\lambda-\mu|-1}(\cos\beta/2)^{|\lambda+\mu|-1} \\ & \times \left[\frac{(j-\lambda)!(j-\mu-1)!}{(j+\lambda)!(j+\mu+1)!}\right]^{1/2} \Big\{[(\mu-\lambda)-|\mu-\lambda|](1+\cos\beta) \\ & - [(\mu+\lambda)-|\mu+\lambda|](1-\cos\beta)2\sin^2\beta\frac{d}{d\cos\beta}\Big\} \\ & \times P^j_{\lambda,\mu}(\cos\beta). \end{aligned} \tag{A1.10}$$

Now, the symmetry properties (A1.4) and (A1.5) imply that we only require expressions for $d^j_{\lambda\mu}$ for positive values of λ and μ. And (A1.6) implies that we can, in fact, choose to work with $\lambda \geq \mu \geq 0$. This will turn out to be very helpful since we have simple expressions for $d^j_{\lambda 0}$ when $j = l =$ integer and for $d^j_{\lambda,1/2}$ when $j = l + 1/2 =$ half-integer, and the other $d^l_{\lambda,\mu}$ for $\mu > 0$ or $\mu > 1/2$ can then be built up from these. In

https://doi.org/10.1017/9781009402040.015 Published online by Cambridge University Press

this case (A1.10) becomes a simple recursion formula for the polynomial $P^j_{\lambda,\mu}(\cos\beta)$.

Namely, for $\lambda \geq \mu + 1 \geq 1$ on the left-hand side one has:

$$P^j_{\lambda,\mu+1}(\cos\beta) = \left(\mu - \lambda + (1-\cos\beta)\frac{d}{d\cos\beta}\right) P^j_{\lambda,\mu}(\cos\beta). \tag{A1.11}$$

The starting functions $P^j_{\lambda 0}$ or $P^j_{\lambda 1/2}$ are obtained as follows.

For $j = l =$ integer one has, for $\lambda \geq 0$,

$$\begin{aligned} d^l_{\lambda 0}(\beta) = {} & (\sin\beta/2)^\lambda (\cos\beta/2)^\lambda (-2)^\lambda \\ & \times \sqrt{\frac{(l-\lambda)!}{(l+\lambda)!}} \frac{d^\lambda}{d\cos\beta^\lambda} P_l(\cos\beta) \end{aligned} \tag{A1.12}$$

where $P_l(\cos\beta)$ are the usual Legendre polynomials. Via (A1.9) we then have, for $\lambda \geq 0$

$$P^l_{\lambda 0}(\cos\beta) = (-2)^\lambda \frac{d^\lambda}{d\cos\beta^\lambda} P_l(\cos\beta). \tag{A1.13}$$

For $j = l + 1/2 =$ half-integer, one can start with the relation given in Jacob and Wick (1959)

$$\begin{aligned} d^j_{\lambda,1/2}(\beta) = {} & \frac{1}{\sqrt{j+1/2}} \left\{ \sqrt{j+\lambda}\cos\beta/2 \; d^l_{\lambda-1/2,0}(\beta) \right. \\ & \left. + \sqrt{j-\lambda}\sin\beta/2 \; d^j_{\lambda+1/2,0}(\beta) \right\}, \end{aligned} \tag{A1.14}$$

which using (A1.9), can be rewritten, for $\lambda \geq 1/2$, $j = l + 1/2$, as

$$\begin{aligned} P^j_{\lambda,1/2}(\cos\beta) = {} & (j+\lambda) P^l_{\lambda-1/2,0}(\cos\beta) \\ & + \frac{1-\cos\beta}{2} P^l_{\lambda+1/2,0}(\cos\beta). \end{aligned} \tag{A1.15}$$

Thus starting with (A1.13) or (A1.15) one can build up the required $P^j_{\lambda,\mu}(\cos\beta)$, from which the d-functions are obtained via (A1.9). In this approach all the d-functions appear with the correct angular factors explicit.

We list a few of the most often used d-functions.

- $j = 1/2$

$$d^{1/2}_{1/2,1/2}(\beta) = \cos\beta/2 \tag{A1.16}$$

- $j = 1$

$$d^1_{11}(\beta) = \frac{1+\cos\beta}{2} \qquad d^1_{10}(\beta) = -\frac{\sin\beta}{\sqrt{2}} \tag{A1.17}$$

$$d^1_{00}(\beta) = \cos\beta \tag{A1.18}$$

https://doi.org/10.1017/9781009402040.015 Published online by Cambridge University Press

- $j = 3/2$

$$d^{3/2}_{3/2,3/2}(\beta) = 6\cos^3\beta/2$$

$$d^{3/2}_{3/2,1/2}(\beta) = -\sqrt{3}(\sin\beta/2)(\cos^2\beta/2) \tag{A1.19}$$

$$d^{3/2}_{1/2,1/2}(\beta) = \tfrac{1}{2}\cos\beta/2(3\cos\beta - 1) \tag{A1.20}$$

- $j = 2$

$$d^2_{22}(\beta) = \frac{1}{4}(1+\cos\beta)^2 \qquad d^2_{21}(\beta) = -\frac{\sin\beta}{2}(1+\cos\beta) \tag{A1.21}$$

$$d^2_{20}(\beta) = \frac{1}{2}\sqrt{\frac{3}{2}}\sin^2\beta \tag{A1.22}$$

$$d^2_{11}(\beta) = \frac{1}{2}(1+\cos\beta)(2\cos\beta - 1) \tag{A1.23}$$

$$d^2_{10}(\beta) = -\sqrt{\frac{3}{2}}\sin\beta\cos\beta \tag{A1.24}$$

$$d^2_{00}(\beta) = \frac{1}{2}(3\cos^2\beta - 1). \tag{A1.25}$$

https://doi.org/10.1017/9781009402040.015 Published online by Cambridge University Press