APPENDIX A

LEGENDRE POLYNOMIALS, ASSOCIATED LEGENDRE FUNCTIONS AND SPHERICAL HARMONICS

A.1. LEGENDRE POLYNOMIALS

Let x be a real variable such that $-1 \leq x \leq 1$. We may also set $x = \cos\theta$, where θ is a real number. The polynomials of degree l

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l, \quad l = 0, 1, 2, \ldots \tag{A.1}$$

are known as the Legendre polynomials. An equivalent definition of $P_l(x)$ can be given in terms of a generating function, namely

$$(1 - 2xs + s^2)^{-1/2} = \sum_{l=0}^{\infty} P_l(x) s^l, \quad |s| < 1 \quad . \tag{A.2}$$

The Legendre polynomials satisfy the differential equation

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + l(l+1)\right] P_l(x) = 0 \quad . \tag{A.3}$$

We have the recurrence relations

$$(2l+1)xP_l - (l+1)P_{l+1} - lP_{l-1} = 0 \quad , \tag{A.4a}$$

$$(x^2-1)\frac{dP_l}{dx} = l(xP_l - P_{l-1}) = \frac{l(l+1)}{2l+1}(P_{l+1} - P_{l-1}) \tag{A.4b}$$

which are also valid for the case $l = 0$ if one defines $P_{-1} = 0$.

The orthogonality relations are

$$\int_{-1}^{+1} P_l(x) P_{l'}(x) dx = \frac{2}{2l+1}\delta_{ll'} \tag{A.5}$$

and the closure relation is given by

$$\frac{1}{2}\sum_{l=0}^{\infty}(2l+1)P_l(x)P_l(x') = \delta(x-x') \quad . \tag{A.6}$$

The Legendre polynomial $P_l(x)$ has the parity $(-)^l$ and has l zeros in the interval $(-1,+1)$. Furthermore,

$$P_l(1) = 1, \quad P_l(-1) = (-1)^l \quad . \tag{A.7}$$

For the lowest values of l the Legendre polynomials are given explicitly by

$$\begin{aligned}
P_0(x) &= 1 \quad , \\
P_1(x) &= x \quad , \\
P_2(x) &= \frac{1}{2}(3x^2-1) \quad , \\
P_3(x) &= \frac{1}{2}(5x^3-3x) \quad , \\
P_4(x) &= \frac{1}{8}(35x^4-30x^2+3) \quad , \\
P_5(x) &= \frac{1}{8}(63x^5-70x^3+15x) \quad .
\end{aligned} \tag{A.8}$$

A.2. ASSOCIATED LEGENDRE FUNCTIONS

The associated Legendre functions $P_l^m(x)$ are defined by the relations

$$P_l^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_l(x), \quad m = 0,1,2,\ldots,l \quad . \tag{A.9}$$

They are the product of the function $(1-x^2)^{m/2}$ and of a polynomial of degree $(l-m)$ and parity $(-)^{l-m}$, having $(l-m)$ zeros in the interval $(-1,+1)$. The functions $P_l^m(x)$ can also be obtained from a generating function, namely

$$(2m-1)!!(1-x^2)^{m/2}s^m(1-2xs+s^2)^{-m-1/2} = \sum_{l=m}^{\infty}P_l^m(x)s^l, \quad |s|<1 \tag{A.10}$$

with

$$\begin{aligned}
(2m-1)!! &= 1.3.5\ldots(2m-1), \quad m = 1,2,\ldots \\
&= 1, \qquad\qquad m = 0 \quad .
\end{aligned} \tag{A.11}$$

In particular, we have

$$P_l^0(x) = P_l(x) \quad , \tag{A.12}$$

$$P_l^l(x) = (2l-1)!!(1-x^2)^{l/2}. \tag{A.13}$$

The associated Legendre functions satisfy the differential equation

$$\left[(1-x^2)\frac{d^2}{dx^2} - 2x\frac{d}{dx} + l(l+1) - \frac{m^2}{1-x^2}\right] P_l^m(x) = 0 \quad . \tag{A.14}$$

We also have the recurrence relations

$$(2l+1)xP_l^m - (l-m+1)P_{l+1}^m - (l+m)P_{l-1}^m = 0 \quad , \tag{A.15}$$

$$\begin{aligned}(x^2-1)\frac{dP_l^m}{dx} &= -(l+1)xP_l^m + (l-m+1)P_{l+1}^m \\ &= lxP_l^m - (l+m)P_{l-1}^m, \quad 0 \le m \le l-1 \quad ,\end{aligned} \tag{A.16}$$

$$\begin{aligned}P_l^{m+2} - 2(m+1)\frac{x}{(1-x^2)^{1/2}}P_l^{m+1} + (l-m)(l+m+1)P_l^m = 0 \quad , \\ 0 \le m \le l-2 \quad ,\end{aligned} \tag{A.17}$$

$$P_{l-1}^m - P_{l+1}^m = -(2l+1)(1-x^2)^{1/2}P_l^{m-1} \quad , \quad 0 \le m \le l-1 \tag{A.18}$$

and the orthogonality relations

$$\int_{-1}^{+1} P_l^m(x)P_{l'}^m(x)dx = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{ll'}. \tag{A.19}$$

Important particular values are

$$P_l^m(1) = P_l^m(-1) = 0, \quad m \neq 0 \tag{A.20}$$

[for $m = 0$, see eq. (A.7)] and

$$\begin{aligned}P_l^m(0) &= (-)^s\frac{(2s+2m)!}{2^l s!(s+m)!}, \quad & l-m = 2s \\ &= 0, & l-m = 2s+1 \quad .\end{aligned} \tag{A.21}$$

The first few associated Legendre functions are given by

$$\begin{aligned}P_1^1(x) &= (1-x^2)^{1/2} \quad , \\ P_2^1(x) &= 3(1-x^2)^{1/2}x \quad , \\ P_2^2(x) &= 3(1-x^2) \quad , \\ P_3^1(x) &= \frac{3}{2}(1-x^2)^{1/2}(5x^2-1) \quad , \\ P_3^2(x) &= 15x(1-x^2) \quad , \\ P_3^3(x) &= 15(1-x^2)^{3/2} \quad .\end{aligned} \tag{A.22}$$

A.3. ORBITAL ANGULAR MOMENTUM AND SPHERICAL HARMONICS

In classical mechanics the orbital angular momentum of a particle is given by

$$\boldsymbol{l} = \mathbf{r} \times \mathbf{p} \tag{A.23}$$

where $\mathbf{r}$ and $\mathbf{p}$ are the position and momentum vectors of the particle, respectively. In wave mechanics $\mathbf{p}$ is represented by the operator $-i\boldsymbol{\nabla}$ (with $\hbar = 1$) so that $\boldsymbol{l}$ is represented by the operator $-i(\mathbf{r} \times \boldsymbol{\nabla})$. The Cartesian components of $\boldsymbol{l}$ are therefore given by

$$\begin{aligned} l_x &= yp_z - zp_y = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ l_y &= zp_x - xp_z = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ l_z &= xp_y - yp_x = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \quad . \end{aligned} \tag{A.24}$$

Using the rules of commutator algebra, together with the basic commutation relations

$$[x, p_x] = [y, p_y] = [z, p_z] = i \tag{A.25}$$

we find that the operators l_x, l_y and l_z satisfy the characteristic commutation relations of angular momenta, namely

$$[l_x, l_y] = il_z, \quad [l_y, l_z] = il_x, \quad [l_z, l_x] = il_y \quad . \tag{A.26}$$

Thus the three operators l_x, l_y, l_z do not mutually commute. However, if we consider the operator

$$\boldsymbol{l}^2 = l_x^2 + l_y^2 + l_z^2 \tag{A.27}$$

we readily find that each of the operators l_x, l_y and l_z commutes with $\boldsymbol{l}^2$,

$$[l_x, \boldsymbol{l}^2] = [l_y, \boldsymbol{l}^2] = [l_z, \boldsymbol{l}^2] = 0 \quad . \tag{A.28}$$

As a result, it is always possible to construct simultaneous eigenfunctions of $\boldsymbol{l}^2$ and one component of $\boldsymbol{l}$, which we shall choose to be l_z.

Let us use spherical polar coordinates (r, θ, ϕ), with

$$\begin{aligned} x &= r \sin\theta \cos\phi \quad , \\ y &= r \sin\theta \sin\phi \quad , \\ z &= r \cos\theta \quad . \end{aligned} \tag{A.29}$$

We then have

$$l_x = i\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) \quad , \tag{A.30a}$$

$$l_y = i\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \quad , \tag{A.30b}$$

$$l_z = -i\frac{\partial}{\partial\phi} \tag{A.30c}$$

and

$$\boldsymbol{l}^2 = -\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \quad . \tag{A.31}$$

The spherical harmonics $Y_{lm}(\theta,\phi)$ are simultaneous eigenfunctions of the operators $\boldsymbol{l}^2$ and l_z. That is (with $\hbar = 1$)

$$\boldsymbol{l}^2 Y_{lm} = l(l+1)Y_{lm}, \qquad l = 0, 1, 2, \ldots \tag{A.32}$$

$$l_z Y_{lm} = mY_{lm}, \qquad m = -l, -l+1, \ldots, l \quad . \tag{A.33}$$

They are given by

$$Y_{lm}(\theta,\phi) = (-1)^m\left[\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right]^{1/2} P_l^m(\cos\theta)\exp(im\phi), \tag{A.34a}$$
$m \geq 0$

$$Y_{l,-m}(\theta,\phi) = (-1)^m Y_{lm}^*(\theta,\phi) \tag{A.34b}$$

and have the parity $(-)^l$. Hence, in a reflection about the origin such that $(\theta,\phi) \to (\pi-\theta, \phi+\pi)$, we have

$$Y_{lm}(\pi-\theta, \phi+\pi) = (-1)^l Y_{lm}(\theta,\phi) \quad . \tag{A.35}$$

The spherical harmonics satisfy the orthonormality relations

$$\begin{aligned}\int Y_{l'm'}^*(\theta,\phi)Y_{lm}(\theta,\phi)d\Omega &\equiv \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta Y_{l'm'}^*(\theta,\phi)Y_{lm}(\theta,\phi) \\ &= \delta_{ll'}\delta_{mm'}\end{aligned} \tag{A.36}$$

where we have written $d\Omega = \sin\theta d\theta d\phi$. The closure relation for the Y_{lm} is

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{+l} Y_{lm}^*(\theta,\phi)Y_{lm}(\theta',\phi') = \delta(\Omega-\Omega') \tag{A.37a}$$

with

$$\delta(\Omega - \Omega') = \frac{\delta(\theta - \theta')\delta(\phi - \phi')}{\sin\theta} \quad . \tag{A.37b}$$

The spherical harmonics constitute a complete orthonormal set of functions on the unit sphere.

The Y_{lm} also satisfy recurrence relations. Introducing the operators

$$l_\pm = l_x \pm i l_y = \exp(\pm i\phi)\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right) \tag{A.38}$$

we have

$$l_\pm Y_{lm} = [l(l+1) - m(m\pm 1)]^{1/2} Y_{l,m\pm 1} \quad , \tag{A.39a}$$

$$= [(l\mp m)(l+1\pm m)]^{1/2} Y_{l,m\pm 1} \quad , \tag{A.39b}$$

$$l_+ Y_{l,l} = 0 \quad , \tag{A.39c}$$

$$l_- Y_{l,-l} = 0 \tag{A.39d}$$

and also

$$\cos\theta\ Y_{lm} = \left[\frac{(l+1+m)(l+1-m)}{(2l+1)(2l+3)}\right]^{1/2} Y_{l+1,m} + \left[\frac{(l+m)(l-m)}{(2l+1)(2l-1)}\right]^{1/2} Y_{l-1,m}. \tag{A.40}$$

For $m = 0$ and $m = l$ the spherical harmonics are given by the simple expressions

$$Y_{l,0}(\theta,\phi) = \left(\frac{2l+1}{4\pi}\right)^{1/2} P_l(\cos\theta) \tag{A.41}$$

and

$$Y_{l,l}(\theta,\phi) = (-1)^l \left[\frac{2l+1}{4\pi}\frac{(2l)!}{2^{2l}(l!)^2}\right]^{1/2} \sin^l\theta \exp(il\phi) \quad . \tag{A.42}$$

It should be noted that the equations (A.32),(A.33) and (A.36) determine the functions $Y_{lm}(\theta,\phi)$ only up to a phase. Since different phase factor conventions exist in the literature, it is important to carefully check this point in dealing with the functions Y_{lm} used by various authors. The phase of the Y_{lm} is chosen here so that:

1) the functions Y_{lm} verify the recurrence relations (A.39)
2) $Y_{l,0}(\theta = 0)$ is real and positive.

The first few spherical harmonics are given by

$$
\begin{aligned}
Y_{00} &= (4\pi)^{-1/2} \quad , \\
Y_{1,0} &= \left(\frac{3}{4\pi}\right)^{1/2} \cos\theta \quad , \\
Y_{1,\pm1} &= \mp \left(\frac{3}{8\pi}\right)^{1/2} \sin\theta \exp(\pm i\phi) \quad , \\
Y_{2,0} &= \left(\frac{5}{16\pi}\right)^{1/2} (3\cos^2\theta - 1) \quad , \\
Y_{2,\pm1} &= \mp \left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta \exp(\pm i\phi) \quad , \\
Y_{2,\pm2} &= \left(\frac{15}{32\pi}\right)^{1/2} \sin^2\theta \exp(\pm 2i\phi) \quad , \\
Y_{3,0} &= \left(\frac{7}{16\pi}\right)^{1/2} (5\cos^3\theta - 3\cos\theta) \quad , \\
Y_{3,\pm1} &= \mp \left(\frac{21}{64\pi}\right)^{1/2} \sin\theta(5\cos^2\theta - 1)\exp(\pm i\phi) \quad , \\
Y_{3,\pm2} &= \left(\frac{105}{32\pi}\right)^{1/2} \sin^2\theta\cos\theta \exp(\pm 2i\phi) \quad , \\
Y_{3,\pm3} &= \mp \left(\frac{35}{64\pi}\right)^{1/2} \sin^3\theta \exp(\pm 3i\phi) \quad .
\end{aligned}
\tag{A.43}
$$

A.4. USEFUL FORMULAE

Let $\mathbf{r}_1$ and $\mathbf{r}_2$ be two vectors having polar angles (θ_1, ϕ_1) and (θ_2, ϕ_2), respectively, and let θ be the angle between them. The "addition (or biaxial) theorem" of the spherical harmonics states that

$$P_l(\cos\theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y^*_{lm}(\theta_1, \phi_1) Y_{lm}(\theta_2, \phi_2) \tag{A.44a}$$

or

$$P_l(\cos\theta) = \frac{4\pi}{2l+1} \sum_{m=-l}^{+l} Y^*_{lm}(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \tag{A.44b}$$

where $\hat{\mathbf{x}}$ denotes the polar angles of a vector $\mathbf{x}$.

Using the generating function of the Legendre polynomials [see eq. (A.2)] we also see that

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{(r_<)^l}{(r_>)^{l+1}} P_l(\cos\theta) \tag{A.45}$$

where $r_<$ is the smaller and $r_>$ the larger of r_1 and r_2. This result may also be written with the help of eq. (A.44b) as

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{4\pi}{2l+1} \frac{(r_<)^l}{(r_>)^{l+1}} Y^*_{lm}(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2). \tag{A.46}$$

We also have

$$\frac{\exp(ik|\mathbf{r}_1 - \mathbf{r}_2|)}{|\mathbf{r}_1 - \mathbf{r}_2|} = ik \sum_{l=0}^{\infty} (2l+1) j_l(kr_<) h_l^{(1)}(kr_>) P_l(\cos\theta) \tag{A.47a}$$

$$= 4\pi ik \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} j_l(kr_<) h_l^{(1)}(kr_>) Y^*_{lm}(\hat{\mathbf{r}}_1) Y_{lm}(\hat{\mathbf{r}}_2) \tag{A.47b}$$

where j_l and $h_l^{(1)}$ are respectively a spherical Bessel function and a spherical Hankel function of the first kind (see Appendix B).

The development in spherical harmonics of a plane wave $\exp(i\mathbf{k}.\mathbf{r})$ is given by

$$\exp(i\mathbf{k}.\mathbf{r}) = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} i^l j_l(kr) Y^*_{lm}(\hat{\mathbf{k}}) Y_{lm}(\hat{\mathbf{r}}) \tag{A.48}$$

Using the addition theorem (A.44), we may also write

$$\exp(i\mathbf{k}.\mathbf{r}) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) \tag{A.49}$$

where θ is the angle between the vectors $\mathbf{k}$ and $\mathbf{r}$. In particular, if we choose the z-axis to coincide with the direction of $\mathbf{k}$, we have

$$\exp(i\mathbf{k}.\mathbf{r}) = \exp(ikz) = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta) \tag{A.50}$$

It may also be shown (see for example Edmonds, 1957) that

$$\begin{aligned} &\int Y_{l_1 m_1}(\theta,\phi) Y_{l_2 m_2}(\theta,\phi) Y_{l_3 m_3}(\theta,\phi) d\Omega \\ &= \left[\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right]^{1/2} \\ &\times \begin{pmatrix} l_1 & l_2 & l_3 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \end{aligned} \tag{A.51}$$

where we have introduced the Wigner $3-j$ symbols (see Appendix E). From eq. (A.51) we find that

$$
\begin{aligned}
Y_{l_1 m_1}(\theta,\phi) Y_{l_2 m_2}(\theta,\phi) = & \sum_{L=|l_1-l_2|}^{l_1+l_2} \sum_{M=-L}^{+L} (-1)^M \\
& \times \left[\frac{(2l_1+1)(2l_2+1)(2L+1)}{4\pi}\right]^{1/2} \\
& \times \begin{pmatrix} l_1 & l_2 & L \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & M \end{pmatrix} Y_{L,-M}(\theta,\phi)
\end{aligned}
\tag{A.52}
$$

This last equation may also be written in terms of vector addition (or Clebsch–Gordan) coefficients (see Appendix E) as

$$
\begin{aligned}
Y_{l_1 m_1}(\theta,\phi) Y_{l_2 m_2}(\theta,\phi) = & \sum_{L=|l_1-l_2|}^{l_1+l_2} \sum_{M=-L}^{+L} \left[\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}\right]^{1/2} \\
& \times (l_1 0 l_2 0|L0)(l_1 m_1 l_2 m_2|LM) Y_{LM}(\theta,\phi)
\end{aligned}
\tag{A.53}
$$

We remark that in eqs. (A.52) and (A.53), the summation over M reduces to one term with $M = m_1 + m_2$.

Additional useful formulae may be found for example in Abramowitz and Stegun (1964, Chapter 8), Rose (1957) and Edmonds (1957).

APPENDIXB

BESSEL FUNCTIONS, MODIFIED BESSEL FUNCTIONS, SPHERICAL BESSEL FUNCTIONS AND RELATED FUNCTIONS

B.1. BESSEL FUNCTIONS

Let us consider the differential equation

$$z^2\frac{d^2w}{dz^2} + z\frac{dw}{dz} + (z^2 - \nu^2)w = 0 \tag{B.1}$$

where ν is a parameter which is assumed to be real. The so-called cylindrical functions are solutions of this equation. Special cylindrical functions are the Bessel functions $J_\nu(z)$ [also called Bessel functions of the first kind], the Neumann functions $N_\nu(z)$ [also called Bessel functions of the second kind and sometimes denoted $Y_\nu(z)$] and the Hankel functions $H_\nu^{(1)}(z), H_\nu^{(2)}(z)$ [also called Bessel functions of the third kind]. These functions may be defined by the following relations (Abramowitz and Stegun, 1964, Chapter 9; Watson, 1966)

$$J_\nu(z) = (z/2)^\nu \sum_{k=0}^{\infty} \frac{(-z^2/4)^k}{k!\Gamma(\nu+k+1)}, \quad |\arg z| < \pi \tag{B.2}$$

where Γ is the Gamma-function,

$$N_\nu(z) = \frac{1}{\sin(\nu\pi)}[\cos(\nu\pi)J_\nu(z) - J_{-\nu}(z)], \ \nu \neq 0, \pm1, \pm2, \ldots;$$
$$|\arg z| < \pi, \tag{B.3}$$

$$N_n(z) = \lim_{\nu \longrightarrow n} N_\nu(z), \quad n = 0, \pm1, \pm2, \ldots; |\arg z| < \pi, \tag{B.4}$$

$$J_{-n}(z) = (-1)^n J_n(z); N_{-n}(z) = (-1)^n N_n(z), \ n = 0, 1, 2, \ldots \ , \tag{B.5}$$

$$H_\nu^{(1)}(z) = J_\nu(z) + iN_\nu(z), \tag{B.6}$$

$$H_\nu^{(2)}(z) = J_\nu(z) - iN_\nu(z) \quad . \tag{B.7}$$

The functions pairs $\{J_\nu(z), N_\nu(z)\}$ and $\{H_\nu^{(1)}(z), H_\nu^{(2)}(z)\}$ are linearly independent solutions of eq. (B.1) for all values of ν.

We also note the integral representations

$$J_\nu(z) = \frac{1}{\pi}\int_0^\pi \cos(z\sin\phi - \nu\phi)d\phi - \frac{\sin(\nu\pi)}{\pi}\int_0^\infty \exp(-z\sinh t - \nu t)dt,$$
$$|\arg z| < \pi/2, \tag{B.8a}$$

$$\begin{aligned} N_\nu(z) = &\frac{1}{\pi}\int_0^\pi \sin(z\sin\phi - \nu\phi)d\phi \\ &- \frac{1}{\pi}\int_0^\infty [\exp(\nu t) + \exp(-\nu t)\cos(\nu\pi)]\exp(-z\sinh t)dt, \\ &|\arg z| < \pi/2 \end{aligned} \tag{B.8b}$$

and

$$\begin{aligned} J_n(z) &= \frac{1}{\pi}\int_0^\pi \cos(z\sin\phi - n\phi)d\phi \\ &= \frac{i^{-n}}{\pi}\int_0^\pi \exp(iz\cos\phi)\cos(n\phi)d\phi, \;\; n = 0, 1, 2, \ldots \quad . \end{aligned} \tag{B.8c}$$

If C denotes $J, N, H^{(1)}, H^{(2)}$ or any linear combination of these functions (the coefficients of which are independent of z and ν) we have the recurrence relations

$$C_{\nu-1}(z) + C_{\nu+1}(z) = \frac{2\nu}{z}C_\nu(z) \quad , \tag{B.9a}$$

$$C_{\nu-1}(z) - C_{\nu+1}(z) = 2\frac{dC_\nu(z)}{dz} \quad , \tag{B.9b}$$

$$\frac{dC_\nu(z)}{dz} = C_{\nu-1}(z) - \frac{\nu}{z}C_\nu(z) \quad , \tag{B.9c}$$

$$\frac{dC_\nu(z)}{dz} = -C_{\nu+1}(z) - \frac{\nu}{z}C_\nu(z) \quad . \tag{B.9d}$$

We also have

$$\frac{dJ_0(z)}{dz} = -J_1(z); \quad \frac{dN_0(z)}{dz} = -N_1(z) \tag{B.9e}$$

A generating function for the Bessel functions is given by

$$\exp\left[\frac{z}{2}\left(t-\frac{1}{t}\right)\right] = \sum_{k=-\infty}^{+\infty} t^k J_k(z) \ , \quad t \neq 0 \quad . \tag{B.10}$$

When ν is fixed and $z \to 0$, we have

$$J_\nu(z) \underset{z\to 0}{\to} \frac{(z/2)^\nu}{\Gamma(\nu+1)} \qquad (\nu \neq -1,-2,-3,\ldots) \tag{B.11a}$$

$$N_0(z) \underset{z\to 0}{\to} \frac{2}{\pi}\ln z \tag{B.11b}$$

$$N_\nu(z) \underset{z\to 0}{\to} -\frac{\Gamma(\nu)}{\pi}(z/2)^{-\nu}, \quad \mathrm{Re}\ \nu > 0 \quad . \tag{B.11c}$$

For ν fixed and $|z| \to \infty$ we have the asymptotic expressions

$$J_\nu(z) \underset{|z|\to\infty}{\to} \left(\frac{2}{\pi z}\right)^{1/2} \cos\left(z-\frac{\nu\pi}{2}-\frac{\pi}{4}\right), \quad |\arg z| < \pi, \tag{B.12a}$$

$$N_\nu(z) \underset{|z|\to\infty}{\to} \left(\frac{2}{\pi z}\right)^{1/2} \sin\left(z-\frac{\nu\pi}{2}-\frac{\pi}{4}\right), \quad |\arg z| < \pi, \tag{B.12b}$$

$$H_\nu^{(1)}(z) \underset{|z|\to\infty}{\to} \left(\frac{2}{\pi z}\right)^{1/2} \exp\left[i\left(z-\frac{\nu\pi}{2}-\frac{\pi}{4}\right)\right], -\pi < \arg z < 2\pi, \tag{B.12c}$$

$$H_\nu^{(2)}(z) \underset{|z|\to\infty}{\to} \left(\frac{2}{\pi z}\right)^{1/2} \exp\left[-i\left(z-\frac{\nu\pi}{2}-\frac{\pi}{4}\right)\right], -2\pi < \arg z < \pi. \tag{B.12d}$$

B.2. MODIFIED BESSEL FUNCTIONS

Let us now consider the differential equation

$$z^2\frac{d^2w}{dz^2} + z\frac{dw}{dz} - (z^2+\nu^2)w = 0 \tag{B.13}$$

The modified cylindrical functions are solutions of this equation. Particular modified cylindrical functions are the modified Bessel functions $I_\nu(z)$ and $K_\nu(z)$ such that

$$I_\nu(z) = \exp(-\nu\pi i/2)J_\nu[z\exp(i\pi/2)], \quad -\pi < \arg z \leq \frac{\pi}{2} \tag{B.14a}$$

$$= \exp(3\nu\pi i/2)J_\nu[z\exp(-3i\pi/2)], \quad \frac{\pi}{2} < \arg z \leq \pi \tag{B.14b}$$

and

$$K_\nu(z) = \frac{\pi i}{2}\exp(\nu\pi i/2)H_\nu^{(1)}[z\exp(i\pi/2)], \quad -\pi < \arg z \le \frac{\pi}{2} \quad \text{(B.15a)}$$

$$= -\frac{\pi i}{2}\exp(-\nu\pi i/2)H_\nu^{(2)}[z\exp(-i\pi/2)], \quad -\frac{\pi}{2} < \arg z \le \pi \ . \quad \text{(B.15b)}$$

We also have

$$I_\nu(z) = (z/2)^\nu \sum_{k=0}^{\infty} \frac{(z^2/4)^k}{k!\Gamma(\nu+k+1)} \quad \text{(B.16)}$$

$$K_\nu(z) = \frac{\pi}{2\sin(\nu\pi)}[I_{-\nu}(z) - I_\nu(z)], \quad \nu \ne 0, \pm 1, \pm 2, \dots \quad \text{(B.17)}$$

$$K_n(z) = \lim_{\nu \to n} K_\nu(z) \ , \quad n = 0, \pm 1, \pm 2, \dots \quad \text{(B.18)}$$

$$K_0(z) = -\{\ln(z/2) + \gamma\} I_0(z) + \frac{z^2/4}{(1!)^2} + \left(1 + \frac{1}{2}\right)\frac{(z^2/4)^2}{(2!)^2} + \left(1 + \frac{1}{2} + \frac{1}{3}\right)\frac{(z^2/4)^3}{(3!)^2} + \dots \quad \text{(B.19)}$$

where $\gamma = 0.5772156649\dots$ is Euler's constant,

$$I_{-n}(z) = I_n(z), \quad n = 0, 1, 2, \dots \quad \text{(B.20)}$$

$$K_{-\nu}(z) = K_\nu(z) \quad . \quad \text{(B.21)}$$

We also note the integral representations

$$I_\nu = \frac{1}{\pi}\int_0^\pi \exp(z\cos\phi)\cos(\nu\phi)d\phi - \frac{\sin(\nu\pi)}{\pi}\int_0^\infty \exp(-z\cosh t - \nu t)dt \ , \quad |\arg z| < \frac{\pi}{2} \quad \text{(B.22a)}$$

$$K_\nu(z) = \int_0^\pi \exp(-z\cosh t)\cosh(\nu t)dt, \quad |\arg z| < \frac{\pi}{2} \ , \quad \text{(B.22b)}$$

$$K_\nu(z) = \frac{\pi^{1/2}(z/2)^\nu}{\Gamma\left(\nu + \frac{1}{2}\right)}\int_1^\infty \frac{\exp(-zt)}{(t^2-1)^{1/2-\nu}}dt, \quad \text{Re } \nu > -\frac{1}{2}, \ |\arg z| < \frac{\pi}{2} \ . \quad \text{(B.22c)}$$

In particular,

$$K_0(z) = \int_1^\infty \frac{\exp(-zt)}{(t^2-1)^{1/2}}dt = \int_0^\infty \frac{\exp[-z(u^2+1)^{1/2}]}{(u^2+1)^{1/2}}du, \qquad |\arg z| < \frac{\pi}{2} . \tag{B.22d}$$

If Z denotes $I_\nu, \exp(\nu\pi i)K_\nu$ or any linear combination of these functions (the coefficients of which are independent of z and ν), we have the recurrence relations

$$Z_{\nu-1}(z) - Z_{\nu+1}(z) = \frac{2\nu}{z}Z_\nu(z) \quad , \tag{B.23a}$$

$$\frac{dZ_\nu(z)}{dz} = Z_{\nu-1}(z) - \frac{\nu}{z}Z_\nu(z) \quad , \tag{B.23b}$$

$$Z_{\nu-1}(z) + Z_{\nu+1}(z) = 2\frac{dZ_\nu(z)}{dz} \quad , \tag{B.23c}$$

$$\frac{dZ_\nu(z)}{dz} = Z_{\nu+1}(z) + \frac{\nu}{z}Z_\nu(z) \quad . \tag{B.23d}$$

We also have

$$\frac{dI_0(z)}{dz} = I_1(z); \qquad \frac{dK_0(z)}{dz} = -K_1(z) \quad . \tag{B.23e}$$

When ν is fixed and $z \to 0$,

$$I_\nu(z) \underset{z\to 0}{\to} \frac{(z/2)^\nu}{\Gamma(\nu+1)} \quad (\nu \neq -1, -2, -3, \ldots) \tag{B.24a}$$

$$K_0(z) \underset{z\to 0}{\to} -\ln z \tag{B.24b}$$

$$K_\nu(z) \underset{z\to 0}{\to} \frac{1}{2}\Gamma(\nu)(z/2)^{-\nu} \quad \mathrm{Re}\ \nu > 0 \quad . \tag{B.24c}$$

B.3. SPHERICAL BESSEL FUNCTIONS

Let us consider the differential equation

$$\frac{d^2w}{dz^2} + \frac{2}{z}\frac{dw}{dz} + \left[1 - \frac{l(l+1)}{z^2}\right]w = 0 \tag{B.25}$$

with $l = 0, 1, 2, \ldots$. Particular solutions of this equation are the spherical Bessel functions (or spherical Bessel functions of the first kind)

$$j_l(z) = \left(\frac{\pi}{2z}\right)^{1/2} J_{l+1/2}(z), \tag{B.26}$$

the spherical Neumann functions (or spherical Bessel functions of the second kind)

$$\begin{aligned} n_l(z) &= (-1)^{l+1}\left(\frac{\pi}{2z}\right)^{1/2} J_{-l-1/2}(z) \\ &= \left(\frac{\pi}{2z}\right)^{1/2} N_{l+1/2}(z) \end{aligned} \tag{B.27}$$

and the spherical Hankel functions of the first and second kind

$$\begin{aligned} h_l^{(1)}(z) &= j_l(z) + i n_l(z) \\ &= \left(\frac{\pi}{2z}\right)^{1/2} H_{l+1/2}^{(1)}(z) \end{aligned} \tag{B.28}$$

$$\begin{aligned} h_l^{(2)}(z) &= j_l(z) - i n_l(z) \\ &= \left(\frac{\pi}{2z}\right)^{1/2} H_{l+1/2}^{(2)}(z) \end{aligned} \tag{B.29}$$

The functions $j_l(z)$ are regular while the functions $n_l(z), h_l^{(1)}(z)$ and $h_l^{(2)}(z)$ are irregular at the origin. The functions pairs $\{j_l(z), n_l(z)\}$ and $\{h_l^{(1)}(z), h_l^{(2)}(z)\}$ are linearly independent solutions of eq. (B.25) for every l.

The first three functions $j_l(z)$ and $n_l(z)$ are given explicitly by

$$\begin{aligned} j_0(z) &= \frac{\sin z}{z}\,, \\ j_1(z) &= \frac{\sin z}{z^2} - \frac{\cos z}{z}\,, \\ j_2(z) &= \left(\frac{3}{z^3} - \frac{1}{z}\right)\sin z - \frac{3}{z^2}\cos z\,, \end{aligned} \tag{B.30a}$$

and

$$\begin{aligned} n_0(z) &= -\frac{\cos z}{z}\,, \\ n_1(z) &= -\frac{\cos z}{z^2} - \frac{\sin z}{z}\,, \\ n_2(z) &= -\left(\frac{3}{z^3} + \frac{1}{z}\right)\cos z - \frac{3}{z^2}\sin z\,. \end{aligned} \tag{B.30b}$$

The functions $j_l(z)$ and $n_l(z)$ may be represented by the ascending series

$$\begin{aligned} j_l(z) &= \frac{z^l}{(2l+1)!!} \\ &\times \left[1 - \frac{z^2/2}{1!(2l+3)} + \frac{(z^2/2)^2}{2!(2l+3)(2l+5)} - \dots\right], \end{aligned} \tag{B.31a}$$

$$\begin{aligned} n_l(z) &= -\frac{(2l-1)!!}{z^{l+1}} \\ &\times \left[1 - \frac{z^2/2}{1!(1-2l)} + \frac{(z^2/2)^2}{2!(1-2l)(3-2l)} - \dots\right] \end{aligned} \tag{B.31b}$$

and for l fixed and $z \to 0$ we see that

$$j_l(z) \underset{z\to 0}{\longrightarrow} \frac{z^l}{(2l+1)!!} , \tag{B.32a}$$

$$n_l(z) \underset{z\to 0}{\longrightarrow} -\frac{(2l-1)!!}{z^{l+1}} . \tag{B.32b}$$

For l fixed and real $x \to \infty$ [in fact for x somewhat larger than $l(l+1)/2$] we have the asymptotic formulae

$$j_l(x) \underset{x\to\infty}{\longrightarrow} \frac{1}{x} \sin\left(x - \frac{l\pi}{2}\right) , \tag{B.33a}$$

$$n_l(x) \underset{x\to\infty}{\longrightarrow} -\frac{1}{x} \cos\left(x - \frac{l\pi}{\pi}\right) , \tag{B.33b}$$

$$h_l^{(1)}(x) \underset{x\to\infty}{\longrightarrow} -i\frac{\exp[i(x - l\pi/2)]}{x} , \tag{B.33c}$$

$$h_l^{(2)}(x) \underset{x\to\infty}{\longrightarrow} i\frac{\exp[-i(x - l\pi/2)]}{x} . \tag{B.33d}$$

If f_l denotes $j_l, n_l, h_l^{(1)}$ or $h_l^{(2)}$, we have the recurrence relations (with $l > 0$)

$$f_{l-1}(z) + f_{l+1}(z) = (2l+1)z^{-1}f_l(z) , \tag{B.34a}$$

$$lf_{l-1}(z) - (l+1)f_{l+1}(z) = (2l+1)\frac{d}{dz}f_l(z) , \tag{B.34b}$$

$$\frac{l+1}{z}f_l(z) + \frac{d}{dz}f_l(z) = f_{l-1}(z) , \tag{B.34c}$$

$$\frac{l}{z}f_l(z) - \frac{d}{dz}f_l(z) = f_{l+1}(z) . \tag{B.34d}$$

We also have the differentiation formulae (with $m = 1, 2, 3, \ldots$)

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m [z^{l+1}f_l(z)] = z^{l-m+1}f_{l-m}(z), \tag{B.35a}$$

$$\left(\frac{1}{z}\frac{d}{dz}\right)^m [z^{-l}f_l(z)] = (-1)^m z^{-l-m}f_{l+m}(z) \tag{B.35b}$$

and the additional useful relations

$$j_l(z)n_{l-1}(z) - j_{l-1}(z)n_l(z) = z^{-2}, \quad l > 0, \tag{B.36a}$$

$$j_l(z)\frac{d}{dz}n_l(z) - n_l(z)\frac{d}{dz}j_l(z) = z^{-2} . \tag{B.36b}$$

We also quote the following indefinite integrals

$$\int j_0^2(x)x^2dx = \frac{1}{2}x^3[j_0^2(x) + n_0(x)j_1(x)] \ , \tag{B.37a}$$

$$\int n_0^2(x)x^2dx = \frac{1}{2}x^3[n_0^2(x) - j_0(x)n_1(x)] \ , \tag{B.37b}$$

$$\int j_1(x)dx = -j_0(x) \ , \tag{B.37c}$$

$$\int j_0(x)x^2dx = x^2j_1(x) \ , \tag{B.37d}$$

$$\int j_l^2(x)x^2dx = \frac{1}{2}x^3[j_l^2(x) - j_{l-1}(x)j_{l+1}(x)], \quad l > 0 \ . \tag{B.37e}$$

The following definite integrals involving the functions j_l often appear in electron–atom scattering calculations:

$$\begin{aligned}&\int_0^\infty \exp(-ax)j_l(bx)x^{\mu-1}dx \\ &= \frac{\pi^{1/2}b^l\Gamma(\mu+l)}{2^{l+1}a^{\mu+l}\Gamma(l+3/2)}\ {}_2F_1\left(\frac{\mu+l}{2}, \frac{\mu+l+1}{2}; l+\frac{3}{2}; -\frac{b^2}{a^2}\right), \\ &\mathrm{Re}(a+ib) > 0, \mathrm{Re}(a-ib) > 0, \mathrm{Re}(\mu+l) > 0\end{aligned} \tag{B.38a}$$

where

$${}_2F_1(a,b;c;z) = 1 + \frac{ab}{c}\frac{z}{1!} + \frac{a(a+1)b(b+1)}{c(c+1)}\frac{z^2}{2!} + \ldots \tag{B.38b}$$

is the hypergeometric function,

$$\int_0^\infty \exp(-ax)j_l(bx)x^{l+1}dx = \frac{(2b)^l\Gamma(l+1)}{(a^2+b^2)^{l+1}}, \quad \mathrm{Re}\,a > |\,\mathrm{Im}\,b|, \tag{B.38c}$$

$$\int_0^\infty \exp(-ax)j_l(bx)x^{l+2}dx = \frac{2a(2b)^l\Gamma(l+2)}{(a^2+b^2)^{l+2}}, \quad \mathrm{Re}\,a > |\,\mathrm{Im}\,b|. \tag{B.38d}$$

Similar integrals involving higher powers of x may be obtained by differentiation with respect to the quantity a.

Finally, we remark that

$$\int_0^\infty j_l(kr)j_l(k'r)r^2dr = \frac{\pi}{2k^2}\delta(k-k') \quad . \tag{B.39}$$

Additional useful formulae are given for example in Abramowitz and Stegun (1964, Chapters 9 and 10) and Watson (1966).

APPENDIX C

DALITZ INTEGRALS

In this appendix we shall study integrals of the type (Dalitz, 1951, Joachain, 1983)

$$
\begin{aligned}
&I_{m,n}(\alpha,\beta;\mathbf{k}_i,\mathbf{k}_f;\bar{k}) \\
&= \int d\mathbf{q}\frac{1}{q^2-\bar{k}^2-i\epsilon}\;\frac{1}{[\alpha^2+(\mathbf{q}-\mathbf{k}_i)^2]^m}\;\frac{1}{[\beta^2+(\mathbf{q}-\mathbf{k}_f)^2]^n}
\end{aligned}
\tag{C.1}
$$

with $\epsilon \to 0^+$. Following Feynman (1949), we first set

$$
\begin{aligned}
a &= \alpha^2+(\mathbf{q}-\mathbf{k}_i)^2 \\
b &= \beta^2+(\mathbf{q}-\mathbf{k}_f)^2
\end{aligned}
\tag{C.2}
$$

and use the integral representation

$$
\frac{1}{ab} = \int_0^1 \frac{dt}{[at+b(1-t)]^2}. \tag{C.3a}
$$

By differentiating both sides of eq. (C.3a) with respect to a or (and) b, we also have

$$
\frac{1}{a^2b} = 2\int_0^1 \frac{t}{[at+b(1-t)]^3}dt \quad , \tag{C.3b}
$$

$$
\frac{1}{ab^2} = 2\int_0^1 \frac{1-t}{[at+b(1-t)]^3}dt \quad , \tag{C.3c}
$$

$$\vdots$$

$$
\frac{1}{a^mb^n} = \frac{(m+n-1)!}{(m-1)!(n-1)!}\int_0^1 \frac{t^{m-1}(1-t)^{n-1}}{[at+b(1-t)]^{m+n}}dt \tag{C.3d}
$$

so that we may rewrite eq. (C.1) as

$$I_{m,n}(\alpha,\beta;\mathbf{k}_i,\mathbf{k}_f;\bar{k}) = \frac{(m+n-1)!}{(m-1)!(n-1)!}\int_0^1 dt\ t^{m-1}(1-t)^{n-1}$$
$$\times \int d\mathbf{q}\frac{1}{q^2-\bar{k}^2-i\epsilon} \tag{C.4}$$
$$\times \frac{1}{[\alpha^2 t+(\mathbf{q}-\mathbf{k}_i)^2 t+\beta^2(1-t)+(\mathbf{q}-\mathbf{k}_f)^2(1-t)]^{m+n}} \quad .$$

We now observe that

$$\alpha^2 t+(\mathbf{q}-\mathbf{k}_i)^2 t+\beta^2(1-t)+(\mathbf{q}-\mathbf{k}_f)^2(1-t) = \Gamma^2+(\mathbf{q}-\mathbf{\Lambda})^2 \tag{C.5}$$

where

$$\mathbf{\Lambda} = t\mathbf{k}_i+(1-t)\mathbf{k}_f \quad , \tag{C.6}$$
$$\begin{aligned}\Gamma^2 &= \alpha^2 t+\beta^2(1-t)+t(1-t)(\mathbf{k}_i-\mathbf{k}_f)^2\\ &= \alpha^2 t+\beta^2(1-t)+t(1-t)\Delta^2\end{aligned} \tag{C.7}$$

and we recall that $\mathbf{\Delta}=\mathbf{k}_i-\mathbf{k}_f$ is the momentum transfer.

Apart from a one-dimensional integral on the t variable, the calculation of $I_{m,n}(\alpha,\beta;\mathbf{k}_i,\mathbf{k}_f;\bar{k})$ therefore reduces to the evaluation of integrals of the type

$$L_S = \int d\mathbf{q}\ \frac{1}{q^2-\bar{k}^2-i\epsilon}\ \frac{1}{[\Gamma^2+(\mathbf{q}-\mathbf{\Lambda})^2]^S} \quad . \tag{C.8}$$

Let us begin by considering the case $S=1$. Using spherical coordinates (q,θ_q,ϕ_q) in $\mathbf{q}$ space, taking the z-axis along the vector $\mathbf{\Lambda}$ and performing the integration over the azimuthal angle ϕ_q, we find that

$$L_1 = 2\pi\int_0^\pi d\theta_q\sin\theta_q\int_0^{+\infty} dq q^2$$
$$\frac{1}{q^2-\bar{k}^2-i\epsilon}\times\frac{1}{\Gamma^2+q^2+\Lambda^2-2q\Lambda\cos\theta_q} \quad . \tag{C.9}$$

Upon changing the integration variables in this equation to $q'=-q$ and $\theta_{q'}=\pi-\theta_q$, we can also write

$$L_1 = 2\pi\int_0^\pi d\theta_{q'}\sin\theta_{q'}\int_{-\infty}^0 dq' q'^2$$
$$\times\frac{1}{q'^2-\bar{k}^2-i\epsilon}\ \frac{1}{\Gamma^2+q'^2+\Lambda^2-2q'\Lambda\cos\theta_{q'}} \tag{C.10}$$

so that, by comparing eqs. (C.9) and (C.10), we have

$$L_1 = \pi \int_0^\pi d\theta_q \sin\theta_q \int_{-\infty}^{+\infty} dq q^2 \times \frac{1}{q^2 - \bar{k}^2 - i\epsilon} \frac{1}{\Gamma^2 + q^2 + \Lambda^2 - 2q\Lambda\cos\theta_q} \quad . \tag{C.11}$$

The integral on the q variable may be performed by considering q as a complex variable and closing the contour with a semi-circle of infinite radius in the upper-half complex q-plane. The poles of the denominator in this upper-half q-plane are located at q_1 and q_2, with

$$q_1 = \bar{k} + i\epsilon, \quad q_2 = \Lambda\cos\theta_q + i(\Gamma^2 + \Lambda^2 \sin^2\theta_q)^{1/2} \quad . \tag{C.12}$$

Hence, using the residue theorem, we have

$$L_1 = \pi^2 i\bar{k} \int_{-1}^{+1} \frac{d\omega}{\Gamma^2 + \bar{k}^2 + \Lambda^2 - 2\bar{k}\Lambda\omega} + \frac{\pi^2 i}{\Lambda} \int_{i\Gamma-\Lambda}^{i\Gamma+\Lambda} \frac{q_2}{q_2^2 - \bar{k}^2 - i\epsilon} dq_2 \tag{C.13}$$

where we have set $\omega = \cos\theta_q$ in the first integral. Performing the integrals in eq. (C.13), we obtain

$$L_1(\bar{k}, \Gamma, \Lambda) = \frac{\pi^2 i}{\Lambda} \ln\left(\frac{\bar{k} + \Lambda + i\Gamma}{\bar{k} - \Lambda + i\Gamma}\right) \quad . \tag{C.14}$$

The integrals L_S for $S = 2, 3, \ldots$ may be readily obtained from L_1 by successive differentiations with respect to Γ. Thus we have

$$\begin{aligned} L_2(\bar{k}, \Gamma, \Lambda) &= -\frac{1}{2\Gamma}\frac{\partial}{\partial\Gamma} L_1(\bar{k}, \Gamma, \Lambda) \quad , \\ &= -\frac{\pi^2}{\Gamma(\bar{k}^2 - \Gamma^2 - \Lambda^2 + 2i\bar{k}\Gamma)} \quad , \end{aligned} \tag{C.15a}$$

$$\vdots$$

$$L_S(\bar{k}, \Gamma, \Lambda) = -\frac{1}{2(S-1)\Gamma}\frac{\partial}{\partial\Gamma} L_{S-1}(\bar{k}, \Gamma, \Lambda) \quad . \tag{C.15b}$$

Let us now return to the expression for $I_{m,n}(\alpha, \beta; \mathbf{k}_i, \mathbf{k}_f; \bar{k})$ given by eq. (C.4). In certain cases simple closed form expressions may be obtained for the integration on the variable t. For example, when $m = n = 1$ we have (Lewis, 1956)

$$I_{1,1}(\alpha, \beta; \mathbf{k}_i, \mathbf{k}_f; \bar{k}) = \pi^2 (A^2 - B)^{-1/2} \ln\left[\frac{A + (A^2 - B)^{1/2}}{A - (A^2 - B)^{1/2}}\right] \tag{C.16a}$$

where

$$A = -i\bar{k}[\Delta^2 + (\alpha+\beta)^2] + \alpha(k_f^2 + \beta^2 - \bar{k}^2) + \beta(k_i^2 + \alpha^2 - \bar{k}^2) \quad \text{(C.16b)}$$

and

$$B = [\Delta^2 + (\alpha+\beta)^2][k_i^2 + (\alpha - i\bar{k})^2][k_f^2 + (\beta - i\bar{k})^2] \quad . \quad \text{(C.16c)}$$

It should be noted that the function on the right of eq. (C.16a) is single valued, even when we cross a branch cut of $(A^2 - B)^{1/2}$, i.e. either square root can be chosen. This function is therefore analytic, the only problem being the specification of the branch of the logarithm; examination shows that we must take the arguments of numerator and denominator from $-\pi$ to $+\pi$.

Let us look in more detail at the particular case for which $\alpha = \beta \neq 0$ and $k_i = k_f = \bar{k} = k$. Using eqs. (C.16), we find that

$$\begin{aligned} I_{1,1}(\alpha,\alpha;\mathbf{k}_i,\mathbf{k}_f;k) = {} & \frac{2\pi^2}{\Delta[\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2]^{1/2}} \\ & \times \left\{ \tan^{-1} \frac{\alpha\Delta}{2[\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2]^{1/2}} \right. \\ & \left. + \frac{1}{2} i \ln \left[\frac{(\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2)^{1/2} + k\Delta}{(\alpha^4 + 4k^2\alpha^2 + k^2\Delta^2)^{1/2} - k\Delta} \right] \right\} \quad . \end{aligned} \quad \text{(C.17)}$$

We remark that this result may also be obtained by using eqs. (C.4), (C.15a) and the fact that we have here $\Gamma^2 + \Lambda^2 = k^2 + \alpha^2$. Thus we may write

$$I_{1,1}(\alpha,\alpha;\mathbf{k}_i,\mathbf{k}_f;k) = \pi^2 \int_0^1 \frac{dt}{\Gamma(\alpha^2 - 2ik\Gamma)} \quad \text{(C.18)}$$

with $\Gamma = (\alpha^2 + t(1-t)\Delta^2)^{1/2}$. The integral (C.18) is then readily performed in closed form to yield the expression given by eq. (C.17). Substitution of the result (C.17) in eq. (2.37) yields the second Born term (2.38) corresponding to scattering by the Yukawa potential (2.26).

APPENDIX D

THE DENSITY MATRIX

A quantum system is said to be in a pure state when it is completely specified by a single state vector, which is fully determined apart from a constant phase factor. Quantum systems in pure states are prepared by performing a "maximal measurement" or "complete experiment" in which all values of a complete set of commuting observables are determined. Hence pure states represent the ultimate limit of precise observation as allowed by the uncertainty principle; for this reason they are also called states of "maximum knowledge".

In many cases, however, the measurement made on the system is not maximal. For instance, a beam of particles may be prepared in such a way that certain quantum numbers (e.g. the spin orientation) are only known through a probability distribution. Such systems, which cannot be described by a single state vector, are said to be in mixed states. The study of these systems can conveniently be made using the density matrix formalism (von Neumann, 1927; Fano, 1957; ter Haar, 1961; Blum, 1981). This method also presents the advantage of treating pure and mixed systems on the same footing. In this appendix we shall briefly discuss the general properties of the density matrix.

Let us consider a system consisting of an ensemble of N subsystems $\alpha = 1, 2, \ldots, N$. We suppose that each of these subsystems is in a pure state and is therefore characterized by a distinct state vector $\Psi^{(\alpha)}$, which we denote by $|\alpha\rangle$ in the Dirac notation. The state vectors $|\alpha\rangle$ are assumed to be normalized, but need not be orthogonal to each other.

Next, we choose a complete set of basis states $|n\rangle$, namely orthonormal eigenvectors of some complete set of operators. Since these basis states are orthonormal,

$$\langle n'|n\rangle = \delta_{n'n} \text{ or } \delta(n'-n) \tag{D.1}$$

and because they are complete

$$\sum_n |n\rangle\langle n| = 1 \quad . \tag{D.2}$$

Let us expand the pure state $|\alpha\rangle$ in the basis states $|n\rangle$. We have

$$|\alpha\rangle = \sum_n c_n^{(\alpha)} |n\rangle \tag{D.3}$$

with

$$c_n^{(\alpha)} = \langle n|\alpha\rangle \tag{D.4}$$

and

$$\sum_n |c_n^{(\alpha)}|^2 = 1 \quad . \tag{D.5}$$

Consider now an observable represented by an operator A. The expectation value of this operator in the pure state $|\alpha\rangle$ is

$$\begin{aligned}\langle A\rangle_\alpha = \langle\alpha|\,A\,|\alpha\rangle &= \sum_n\sum_{n'} c_{n'}^{(\alpha)*} c_n^{(\alpha)}\,\langle n'|\,A\,|n\rangle \\ &= \sum_n\sum_{n'}\langle n|\alpha\rangle\langle\alpha|n'\rangle\,\langle n'|\,A\,|n\rangle \quad .\end{aligned} \tag{D.6}$$

The average value of A over the ensemble is therefore given by

$$\langle A\rangle = \sum_{\alpha=1}^{N} W_\alpha\,\langle A\rangle_\alpha \tag{D.7}$$

where W_α is the statistical weight of the subsystem α, namely the probability of obtaining this subsystem among the ensemble. The statistical weights W_α must obviously be such that

$$0 \le W_\alpha \le 1 \tag{D.8}$$

and

$$\sum_{\alpha=1}^{N} W_\alpha = 1 \quad . \tag{D.9}$$

Using the result (D.6), we may write eq. (D.7) explicitly as

$$\begin{aligned}\langle A\rangle &= \sum_{\alpha=1}^{N} W_\alpha \sum_n\sum_{n'} c_{n'}^{(\alpha)*} c_n^{(\alpha)}\,\langle n'|\,A\,|n\rangle \\ &= \sum_{\alpha=1}^{N}\sum_n\sum_{n'}\langle n|\alpha\rangle\; W_\alpha\;\langle\alpha|n'\rangle\,\langle n'|\,A\,|n\rangle \quad .\end{aligned} \tag{D.10}$$

Let us now introduce the density operator (or statistical operator) which is defined as

$$\rho = \sum_{\alpha=1}^{N} |\alpha\rangle\, W_\alpha\,\langle\alpha| \quad . \tag{D.11}$$

Taking matrix elements of the density operator between the basis states $|n\rangle$, we obtain the elements of the density matrix in the $\{|n\rangle\}$ representation, namely

$$\begin{aligned}\rho_{nn'} \equiv \langle n|\,\rho\,|n'\rangle &= \sum_{\alpha=1}^{N} \langle n|\alpha\rangle\ W_\alpha\ \langle \alpha|n'\rangle \\ &= \sum_{\alpha=1}^{N} W_\alpha\ c_{n'}^{(\alpha)*} c_n^{(\alpha)} \quad .\end{aligned} \tag{D.12}$$

Returning to eq. (D.10), we see that

$$\begin{aligned}\langle A\rangle &= \sum_n \sum_{n'} \langle n|\,\rho\,|n'\rangle\,\langle n'|\,A\,|n\rangle \\ &= \sum_n \langle n|\,\rho A\,|n\rangle \\ &= \mathrm{Tr}(\rho A)\end{aligned} \tag{D.13}$$

where the symbol Tr denotes the trace. Hence the knowledge of ρ enables us to obtain the statistical average of A. We also remark that if we take A to be the identity operator, we obtain the normalization condition

$$\mathrm{Tr}\,\rho = 1 \quad . \tag{D.14}$$

As seen from its definition (D.11), the density operator ρ is Hermitian, namely

$$\rho = \rho^\dagger \tag{D.15}$$

or

$$\langle n|\,\rho\,|n'\rangle = \langle n'|\,\rho\,|n\rangle^* \quad . \tag{D.16}$$

As a result, the density matrix may always be diagonalized by means of a unitary transformation.

The diagonal elements of the density matrix,

$$\rho_{nn} = \langle n|\,\rho\,|n\rangle = \sum_{\alpha=1}^{N} W_\alpha\ |c_n^{(\alpha)}|^2 \quad , \tag{D.17}$$

have a simple physical interpretation. Indeed, the probability of finding the system in the pure state $|\alpha\rangle$ is W_α and the probability that $|\alpha\rangle$ is to be found in the state $|n\rangle$ is $|c_n^{(\alpha)}|^2$. Thus the diagonal element ρ_{nn} gives the probability of finding a member of the ensemble in the state n. We also note from eqs. (D.8) and (D.17) that

$$\rho_{nn} \geq 0 \tag{D.18}$$

so that ρ is a positive semi-definite operator. Moreover, combining the above result with eq. (D.14), we see that all diagonal elements of the density matrix must be such that

$$0 \leq \rho_{nn} \leq 1 \quad . \tag{D.19}$$

Let us choose a representation $\{k\}$ in which the density matrix is diagonal. In that representation, we clearly have

$$\rho_{kk'} = \rho_{kk}\delta_{kk'} \tag{D.20}$$

where ρ_{kk} is the fraction of the members of the ensemble in the state $|k\rangle$. Moreover, using eqs (D.14) and (D.19), we have

$$\mathrm{Tr}(\rho^2) \leq \mathrm{Tr}\,\rho = 1 \quad . \tag{D.21}$$

This relation remains valid in any representation since the trace is invariant under a unitary transformation. It is worth noting that because the density matrix is Hermitian the result (D.21) may also be written in the form

$$\sum_n \sum_{n'} |\rho_{nn'}|^2 \leq 1 \quad . \tag{D.22}$$

Let us now consider the particular case such that the system is in a pure state $|\lambda\rangle$. Then $W_\alpha = \delta_{\alpha\lambda}$ and we see from eq. (D.11) that the density operator is just

$$\rho^\lambda = |\lambda\rangle\langle\lambda| \quad . \tag{D.23}$$

This is a projection operator onto the state $|\lambda\rangle$, with

$$(\rho^\lambda)^2 = \rho^\lambda \quad . \tag{D.24}$$

Hence, in this case the relation (D.21) becomes

$$\mathrm{Tr}(\rho^\lambda)^2 = \mathrm{Tr}\,\rho^\lambda = 1 \tag{D.25}$$

and eqs. (D.10) and (D.13) reduce to

$$\langle A\rangle = \mathrm{Tr}(\rho^\lambda A) = \langle\lambda| A |\lambda\rangle \quad . \tag{D.26}$$

It is worth noting that the equation $\mathrm{Tr}(\rho^\lambda)^2 = 1$ gives us a criterion for deciding whether a state is pure or not that is invariant under all unitary transformations.

If we choose to work in a representation $\{k\}$ such that ρ^λ is diagonal, we see that

$$\rho^\lambda_{kk'} = \delta_{k\lambda}\delta_{k'\lambda} \tag{D.27}$$

and therefore the only non-vanishing matrix element of ρ^λ is the diagonal element in the λth row and column, which is equal to one. As a result, all the eigenvalues of the pure state density operator ρ^λ are equal to zero, except one which is equal to unity. This last property is independent of the choice of the representation, and may therefore be used to characterize the density matrix of a pure state.

Let us return to the general density operator (D.11) and density matrix (D.12). Until now we have assumed that the pure states $|\alpha\rangle$ were normalized to unity. If this requirement is dropped, then $0 < \mathrm{Tr}\,\rho \neq 1$ and the basic result (D.13) is replaced by

$$\langle A \rangle = \frac{\mathrm{Tr}(\rho A)}{\mathrm{Tr}\,\rho} \quad . \tag{D.28}$$

In the above discussion we have labelled the rows and columns of the density matrix $\rho_{nn'}$ by simple indices n and n'. In general, of course, the symbol n refers to a collection of indices, some of which taking on discrete values while others vary continuously. In many cases, however, we are interested in some particular property of the system (for example the spin). We then omit the dependence on all other variables, keep only the relevant indices and define in that way a reduced density matrix. This is the case for example in Chapter 4, where we discuss the density matrix for a spin -1/2 system.

APPENDIX E

CLEBSCH–GORDAN AND RACAH COEFFICIENTS

In this appendix we summarize the formulae describing the coupling of two or more angular momenta. This leads to the introduction of Clebsch–Gordan and Racah coefficients as well as higher order $3n - j$ symbols. For a complete discussion of these topics reference should be made to specialized monographs on angular momentum such as those by Rose (1957) and by Edmonds (1957).

E.1. CLEBSCH–GORDAN COEFFICIENTS

Let us first consider two independent quantum systems, or parts of a single system, having angular momenta $\mathbf{j}_1$ and $\mathbf{j}_2$ respectively. We denote by $\psi_{j_1 m_1}(1)$ and $\psi_{j_2 m_2}(2)$ the angular momentum eigenfunctions of these systems which diagonalize the square and the z component of the angular momentum. Thus (with $\hbar = 1$)

$$\begin{aligned} \mathbf{j}_1^2 \psi_{j_1 m_1}(1) &= j_1(j_1+1)\psi_{j_1 m_1}(1) \quad , \\ j_{1z}\psi_{j_1 m_1}(1) &= m_1 \psi_{j_1 m_1}(1) \end{aligned} \tag{E.1}$$

where

$$m_1 = -j_1, -j_1+1, \ldots, j_1 \tag{E.2}$$

and

$$\begin{aligned} \mathbf{j}_2^2 \psi_{j_2 m_2}(2) &= j_2(j_2+1)\psi_{j_2 m_2}(2) \quad , \\ j_{2z}\psi_{j_2 m_2}(2) &= m_2 \psi_{j_2 m_2}(2) \end{aligned} \tag{E.3}$$

where

$$m_2 = -j_2, -j_2+1, \ldots, j_2 \quad . \tag{E.4}$$

Here j_{1z} and j_{2z} are the z components of $\mathbf{j}_1$ and $\mathbf{j}_2$ respectively. Simultaneous eigenfunctions of the operators $\mathbf{j}_1^2, j_{1z}, \mathbf{j}_2^2$ and j_{2z} are then given by the tensor products $\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2)$.

We now define the total angular momentum $\mathbf{j}$ of the two systems by

$$\mathbf{j} = \mathbf{j}_1 + \mathbf{j}_2 \tag{E.5}$$

and its z component j_z by

$$j_z = j_{1z} + j_{2z} \tag{E.6}$$

The operators $\mathbf{j}_1^2, \mathbf{j}_2^2, \mathbf{j}^2$ and j_z form a set of commuting operators. Let us denote by $\psi_{j_1 j_2 jm}(1,2)$ the coupled eigenfunctions common to the operators $\mathbf{j}_1^2, \mathbf{j}_2^2, \mathbf{j}^2$ and j_z. These coupled eigenfunctions satisfy

$$\begin{aligned} \mathbf{j}^2 \psi_{j_1 j_2 jm}(1,2) &= j(j+1)\psi_{j_1 j_2 jm}(1,2) \quad , \\ j_z \psi_{j_1 j_2 jm}(1,2) &= m\psi_{j_1 j_2 jm}(1,2) \end{aligned} \tag{E.7}$$

where

$$j = |j_1 - j_2|, \quad |j_1 - j_2| + 1, \ldots, j_1 + j_2 \tag{E.8}$$

and

$$m = -j, -j+1, \ldots, j \quad . \tag{E.9}$$

The $(2j_1+1)(2j_2+1)$ coupled eigenfunctions $\psi_{j_1 j_2 jm}(1,2)$ common to the operators $\mathbf{j}_1^2, \mathbf{j}_2^2, \mathbf{j}^2$ and j_z are related to the $(2j_1+1)(2j_2+1)$ eigenfunctions $\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2)$ common to the operators $\mathbf{j}_1^2, j_{1z}, \mathbf{j}_2^2$ and j_{2z} by the unitarity transformation

$$\psi_{j_1 j_2 jm}(1,2) = \sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | jm) \psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2) \quad . \tag{E.10}$$

The coefficients $(j_1 m_1 j_2 m_2 | jm)$ of this transformation are called vector coupling or Clebsch–Gordan coefficients. These coefficients vanish unless eqs. (E.8) and (E.9) are satisfied and $m = m_1 + m_2$. To define these coefficients unambiguously, the relative phases of the eigenfunctions $\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2)$ and $\psi_{j_1 j_2 jm}(1,2)$ must be specified. We shall adopt here the phase convention of Condon and Shortley (1935) where

$$(j_1 j_1 j_2 j_2 | j_1 + j_2 \; j_1 + j_2) = 1 \quad . \tag{E.11}$$

With this choice of phase the Clebsch–Gordan coefficients are real and satisfy the orthogonality relations

$$\sum_{m_1 m_2} (j_1 m_1 j_2 m_2 | jm)(j_1 m_1 j_2 m_2 | j' m') = \delta_{jj'} \delta_{mm'}, \tag{E.12}$$

which reduces to a single summation since $m_1 + m_2 = m$, and

$$\sum_{jm} (j_1 m_1 j_2 m_2 | jm)(j_1 m'_1 j_2 m'_2 | jm) = \delta_{m_1 m'_1} \delta_{m_2 m'_2} \quad . \tag{E.13}$$

Using eq. (E.13) we can invert eq. (E.10) to yield

$$\psi_{j_1 m_1}(1)\psi_{j_2 m_2}(2) = \sum_j (j_1 m_1 j_2 m_2 | jm) \psi_{j_1 j_2 jm}(1,2) \quad . \tag{E.14}$$

The Clebsch–Gordan coefficients also satisfy the symmetry relations

$$(j_1 m_1 j_2 m_2 | jm) = (-1)^{j_1+j_2-j} (j_1 - m_1 j_2 - m_2 | j - m) \; , \tag{E.15a}$$

$$(j_1 m_1 j_2 m_2 | jm) = (-1)^{j_1+j_2-j} (j_2 m_2 j_1 m_1 | jm) \; , \tag{E.15b}$$

$$\begin{aligned}(j_1 m_1 j_2 m_2 | jm) &= (-1)^{j_2+m_2} \left(\frac{2j+1}{2j_1+1}\right)^{1/2} \\ &\quad \times (j - m j_2 m_2 | j_1 - m_1) \; ,\end{aligned} \tag{E.15c}$$

$$\begin{aligned}(j_1 m_1 j_2 m_2 | jm) &= (-1)^{j_1-m_1} \left(\frac{2j+1}{2j_2+1}\right)^{1/2} \\ &\quad \times (j_1 m_1 j - m | j_2 - m_2) \; .\end{aligned} \tag{E.15d}$$

Further symmetry relations can be obtained by combining these equations.

These symmetry relations can be simplified by introducing the $3-j$ symbols defined by Wigner (1940). These are defined by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1-j_2-m_3} (2j_3+1)^{-1/2} (j_1 m_1 j_2 m_2 | j_3 - m_3) \quad . \tag{E.16}$$

The $3-j$ symbols are invariant for even permutations of the columns and are multiplied by $(-1)^{j_1+j_2+j_3}$ for odd permutations or when the signs of m_1, m_2 and m_3 are changed. Thus

$$\begin{aligned}\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} &= \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix} \\ &= (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix}\end{aligned} \tag{E.17}$$

and

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1+j_2+j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix} \quad . \tag{E.18}$$

The orthogonality relations satisfied by the $3-j$ symbols are

$$\sum_{m_1 m_2} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3' \\ m_1 & m_2 & m_3' \end{pmatrix} = (2j_3+1)^{-1} \delta_{j_3 j_3'} \delta_{m_3 m_3'} \tag{E.19}$$

and

$$\sum_{j_3 m_3} (2j_3+1) \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1' & m_2' & m_3 \end{pmatrix} = \delta_{m_1 m_1'} \delta_{m_2 m_2'} \quad . \tag{E.20}$$

TABLE E.1. Explicit values for the Clebsch–Gordan coefficients $(j_1 m - m_2 \frac{1}{2} m_2 | jm)$

j	$m_2 = \frac{1}{2}$	$m_2 = -\frac{1}{2}$
$j_1 + \frac{1}{2}$	$\left[\frac{j_1 + m + (1/2)}{2j_1 + 1}\right]^{1/2}$	$\left[\frac{j_1 - m + (1/2)}{2j_1 + 1}\right]^{1/2}$
$j_1 - \frac{1}{2}$	$-\left[\frac{j_1 - m + (1/2)}{2j_1 + 1}\right]^{1/2}$	$\left[\frac{j_1 + m + (1/2)}{2j_1 + 1}\right]^{1/2}$

Returning to Clebsch–Gordan coefficients we have the following important relations

$$(j_1 0 j_2 0 | j 0) = 0 \text{ unless } j_1 + j_2 + j_3 \text{ is even} \tag{E.21}$$

and

$$(j_1 m_1 0 0 | jm) = \delta_{j_1 j} \delta_{m_1 m} \quad . \tag{E.22}$$

The Clebsch–Gordan coefficients can be calculated using the orthogonality and the symmetry relations which they satisfy (Edmonds, 1957). Since the general formula is quite complicated we limit ourselves here to giving their values in Tables E.1 and E.2 for the cases of most interest in this monograph when $j_2 = 1/2$ and $j_2 = 1$.

E.2. RACAH COEFFICIENTS

We now consider the addition of three angular momenta $\mathbf{j}_1, \mathbf{j}_2$ and $\mathbf{j}_3$ to form the total angular momentum $\mathbf{j}$ given by

$$\mathbf{j} = \mathbf{j}_1 + \mathbf{j}_2 + \mathbf{j}_3 \quad . \tag{E.23}$$

There is no unique way of carrying out this addition. We may first couple $\mathbf{j}_1$ and $\mathbf{j}_2$ to give the resultant $\mathbf{j}_{12}$ and then couple this to $\mathbf{j}_3$ to give $\mathbf{j}$. Alternatively, we may couple $\mathbf{j}_1$ to the resultant $\mathbf{j}_{23}$ of coupling $\mathbf{j}_2$ and $\mathbf{j}_3$ to give $\mathbf{j}$. Finally, we may couple $\mathbf{j}_1$ and $\mathbf{j}_3$ to give the resultant $\mathbf{j}_{13}$ which is then coupled with $\mathbf{j}_2$ to give $\mathbf{j}$. These three representations are related by unitary transformations which are expressed in terms of Racah coefficients introduced by Racah (1942, 1943).

Let us consider the connection between the first two representations described above which are characterized by the intermediate angular momenta

$$\mathbf{j}_{12} = \mathbf{j}_1 + \mathbf{j}_2 \text{ and } \mathbf{j}_{23} = \mathbf{j}_2 + \mathbf{j}_3 \tag{E.24}$$

where the corresponding eigenfunctions are denoted by

$$\psi_{jm}(j_{12}) \text{ and } \psi_{jm}(j_{23}) \tag{E.25}$$

TABLE E.2. Explicit values for the Clebsch–Gordan coefficients $(j_1 m - m_2 1 m_2 | jm)$

j	$m_2 = 1$	$m_2 = 0$	$m_2 = -1$
$j_1 + 1$	$\left[\frac{(j_1+m)(j_1+m+1)}{(2j_1+1)(2j_1+2)}\right]^{1/2}$	$\left[\frac{(j_1-m+1)(j_1+m+1)}{(2j_1+1)(j_1+1)}\right]^{1/2}$	$\left[\frac{(j_1-m)(j_1-m+1)}{(2j_1+1)(2j_1+2)}\right]^{1/2}$
j_1	$-\left[\frac{(j_1+m)(j_1-m+1)}{2j_1(j_1+1)}\right]^{1/2}$	$\frac{m}{[j_1(j_1+1)]^{1/2}}$	$\left[\frac{(j_1-m)(j_1+m+1)}{2j_1(j_1+1)}\right]^{1/2}$
$j_1 - 1$	$\left[\frac{(j_1-m)(j_1-m+1)}{2j_1(2j_1+1)}\right]^{1/2}$	$-\left[\frac{(j_1-m)(j_1+m)}{j_1(2j_1+1)}\right]^{1/2}$	$\left[\frac{(j_1+m+1)(j_1+m)}{2j_1(2j_1+1)}\right]^{1/2}$

respectively. These two representations are related by the transformation

$$\psi_{jm}(j_{12}) = \sum_{j_{23}} R(j_{23}\ j_{12})\psi_{jm}(j_{23}). \tag{E.26}$$

The Racah coefficient W is defined by the equation

$$R(j_{23}\ j_{12}) = [(2j_{23}+1)(2j_{12}+1)]^{1/2} W(j_1 j_2 j j_3; j_{12} j_{23}) \quad . \tag{E.27}$$

We can derive a relation between the Racah coefficients and the Clebsch–Gordan coefficients by expressing $\psi_{jm}(j_{12})$ and $\psi_{jm}(j_{23})$ in terms of $\psi_{j_1 m_1}$, $\psi_{j_2 m_2}$ and $\psi_{j_3 m_3}$ using eq. (E.10). We obtain

$$\begin{aligned}\psi_{jm}(j_{12}) = &\sum_{m_1 m_{12}} (j_1 m_1 j_2 m_{12} - m_1 | j_{12} m_{12}) \\ &\times (j_{12} m_{12} j_3 m - m_{12} | jm) \psi_{j_1 m_1} \psi_{j_2 m_{12}-m_1} \psi_{j_3 m-m_{12}}\end{aligned} \tag{E.28}$$

and

$$\begin{aligned}\psi_{jm}(j_{23}) = &\sum_{m_2 m_{23}} (j_2 m_2 j_3 m_{23} - m_2 | j_{23} m_{23}) \\ &\times (j_1 m - m_{23} j_{23} m_{23} | jm) \psi_{j_1 m-m_{23}} \psi_{j_2 m_2} \psi_{j_3 m_{23}-m_2} \ .\end{aligned} \tag{E.29}$$

Substituting these results into eq. (E.26) and using eq. (E.27) gives

$$\begin{aligned}\sum_f [(2e+1)(2f+1)]^{1/2} W(abcd;ef)(b\beta d\delta | f\beta+\delta)(a\alpha f\beta+\delta | c\alpha+\beta+\delta) \\ = (a\alpha b\beta | e\alpha+\beta)(e\alpha+\beta d\delta | c\alpha+\beta+\delta)\end{aligned} \tag{E.30a}$$

Also, using the properties of the Clebsch–Gordan coefficients defined by eqs. (E.12) - (E.15) we obtain the following additional relations

$$\begin{aligned}&[(2e+1)(2f+1)]^{1/2} W(abcd;ef)(a\alpha f\beta+\delta | c\alpha+\beta+\delta) \\ &\quad = \sum_\beta (a\alpha b\beta | e\alpha+\beta)(e\alpha+\beta d\delta | c\alpha+\beta+\delta)(b\beta d\delta | f\beta+\delta)\end{aligned} \tag{E.30b}$$

where $\beta+\delta$ is a fixed parameter and

$$\begin{aligned}&[(2e+1)(2f+1)]^{1/2} W(abcd;ef) = \sum_{\alpha\beta} (a\alpha b\beta | e\alpha+\beta) \\ &\times (e\alpha+\beta d\delta | c\alpha+\beta+\delta)(b\beta d\delta | f\beta+\delta)(a\alpha f\beta+\delta | c\alpha+\beta+\delta)\end{aligned} \tag{E.30c}$$

where $\alpha+\beta+\delta$ is a fixed parameter.

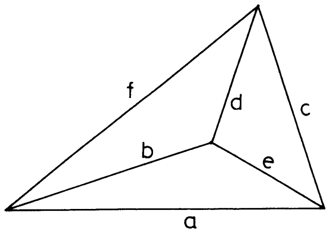

FIGURE E.1. The tetrahedron illustrating the triangular relations satisfied by the arguments of the Racah coefficient $W(abcd;ef)$.

It is clear from the above definitions that the six angular momenta in $W(abcd;ef)$ satisfy the four triangular relations

$$\Delta(abe), \quad \Delta(cde), \quad \Delta(acf), \quad \Delta(bdf) \tag{E.31}$$

where, for example, the notation $\Delta(abe)$ means that the three angular momenta a, b and e form the sides of a triangle. These four triangular relations can be combined by representing the angular momenta by the sides of a tetrahedron as illustrated in figure E.1.

The Racah coefficients also satisfy certain symmetry relations under the twenty-four possible permutations of the six arguments which preserve the four triangular relations. These symmetry relations can be simplified using the $6-j$ symbol introduced by Wigner (1940), which is defined by

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = (-1)^{j_1+j_2+j_4+j_5} W(j_1 j_2 j_5 j_4; j_3 j_6) \quad . \tag{E.32}$$

The $6-j$ symbol is left invariant under any permutations of the three columns. It is also invariant under interchange of the upper and lower arguments in any two columns, e.g.

$$\begin{Bmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{Bmatrix} = \begin{Bmatrix} j_1 & j_5 & j_6 \\ j_4 & j_2 & j_3 \end{Bmatrix} \quad . \tag{E.33}$$

Returning to the Racah coefficients, one can show that they satisfy the orthogonality relation

$$\sum_e (2e+1)(2f+1)W(abcd;ef)W(abcd;eg) = \delta_{fg} \tag{E.34}$$

and the Racah sum rule

$$\sum_e (-1)^{a+b-e}(2e+1)W(abcd;ef)W(bacd;eg) = W(agfb;dc) \quad . \tag{E.35}$$

In addition

$$W(abcd;0f) = \frac{(-1)^{f-b-d}\delta_{ab}\delta_{cd}}{[(2b+1)(2d+1)]^{1/2}} \quad . \tag{E.36}$$

The general closed expression for the Racah coefficient is too complicated to reproduce here but may be found for example in Rose (1957) or Edmonds (1957).

E.3. $9-j$ SYMBOLS

In many applications, we are interested in determining the transformation between two coupling schemes of four angular momenta. This occurs for example in the transformation from LS to jj coupling for two particles possessing both orbital and spin angular momenta. The $9-j$ symbol introduced by Wigner (1940) is defined by the following relation

$$\begin{aligned}&\langle (j_1 j_2) j_{12}, (j_3 j_4) j_{34}, jm | (j_1 j_3) j_{13}, (j_2 j_4) j_{24}, jm \rangle \\ &= [(2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1)]^{1/2} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} .\end{aligned} \tag{E.37}$$

The $9-j$ symbol can be written as the sum over a product of three Racah coefficients by expressing the bra vector in eq. (E.37) in terms of the ket vector in eq. (E.37) by repeated use of the recoupling transformation defined by eqs. (E.26) and (E.27). We find that

$$\begin{aligned}\begin{Bmatrix} j_{11} & j_{12} & j_{13} \\ j_{21} & j_{22} & j_{23} \\ j_{31} & j_{32} & j_{33} \end{Bmatrix} &= \sum_\kappa (-1)^{2\kappa}(2\kappa+1) \begin{Bmatrix} j_{11} & j_{21} & j_{31} \\ j_{32} & j_{33} & \kappa \end{Bmatrix} \\ &\times \begin{Bmatrix} j_{12} & j_{22} & j_{32} \\ j_{21} & \kappa & j_{23} \end{Bmatrix} \begin{Bmatrix} j_{13} & j_{23} & j_{33} \\ \kappa & j_{11} & j_{12} \end{Bmatrix} .\end{aligned} \tag{E.38}$$

An even permutation of the rows or columns of the $9-j$ symbol leaves the symbol unchanged as does the transposition obtained by interchanging rows and columns. An odd transposition of the rows or columns causes the symbol to be multiplied by the factor

$$(-1)^{j_{11}+j_{12}+j_{13}+j_{21}+j_{22}+j_{23}+j_{31}+j_{32}+j_{33}} \quad . \tag{E.39}$$

The $9-j$ symbols also satisfy the orthogonality relation

$$\begin{aligned}&\sum_{j_{12}j_{34}} (2j_{12}+1)(2j_{34}+1)(2j_{13}+1)(2j_{24}+1) \\ &\times \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j'_{13} & j'_{24} & j \end{Bmatrix} = \delta_{j_{13}j'_{13}}\delta_{j_{24}j'_{24}}\end{aligned} \tag{E.40}$$

and the sum rule

$$\sum_{j_{13}j_{24}} (-1)^{2j_2+j_{24}+j_{23}-j_{34}}(2j_{13}+1)(2j_{24}+1)$$
$$\times \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_3 & j_4 & j_{34} \\ j_{13} & j_{24} & j \end{Bmatrix} \begin{Bmatrix} j_1 & j_3 & j_{13} \\ j_4 & j_2 & j_{24} \\ j_{14} & j_{23} & j \end{Bmatrix} = \begin{Bmatrix} j_1 & j_2 & j_{12} \\ j_4 & j_3 & j_{34} \\ j_{14} & j_{23} & j \end{Bmatrix} \tag{E.41}$$

When one argument of a $9-j$ symbol is zero it reduces to a $6-j$ symbol times a factor. As an example we have

$$\begin{Bmatrix} a & b & e \\ c & d & e \\ f & f & 0 \end{Bmatrix} = \frac{(-1)^{b+c+e+f}}{[(2e+1)(2f+1)]^{1/2}} \begin{Bmatrix} a & b & e \\ d & c & f \end{Bmatrix} . \tag{E.42}$$

The corresponding results when the zero appears in one of the other positions can be obtained using the symmetry properties of the $9-j$ symbols discussed above.

E.4. HIGHER ORDER $3n-j$ SYMBOLS

In the theory of electron collisions with complex atoms, $3n-j$ symbols with $n \geq 4$ often arise involving the recoupling of more than four angular momenta. These recoupling coefficients can be expressed as sums over products of Racah coefficients by repeated use of eqs. (E.26) and (E.27) in the same way as eq. (E.38) for the $9-j$ symbol was derived. We shall not discuss here the detailed properties of these higher order $3n-j$ symbols. We remark, however, that a computer code NJSYM has been written by Burke (1970) which enables a general recoupling coefficient for an arbitrary number of angular momenta to be calculated. This code has been incorporated into a number of atomic structure and electron atom collision program packages.

References

ABARBANEL, H. D. I. AND ITZYKSON, C., 1969, *Phys. Rev. Lett.* **23**, 53.
ABDULLAH, J. AND TRUHLAR, D. G., 1974, *J. Chem. Phys.* **60**, 4670.
ABRAMOWITZ, M. AND STEGUN, I. A., 1964, *Handbook of Mathematical Functions* (Dover, New York).
ADHIKARI, S. K., 1974, *Phys. Rev. C* **10**, 1623.
ADHIKARI, S. K. AND SLOAN, I. H., 1975, *Phys. Rev. C* **11**, 1133.
BALUJA, K. L., BURKE, P. G. AND MORGAN, L. A., 1982, *Comput. Phys. Commun.* **27**, 299.
BARGMANN, V., 1949, *Rev. Mod. Phys.* **21**, 488.
BARGMANN, V., 1952, *Proc. Nat. Acad. Sc. U. S.* **38**, 961.
BARRETT, R. F., BIEDENHARN, L. C., DANOS, M., DELSANTO, P. P., GREINER, W. AND WAHSWEILER, H. G., 1973, *Rev. Mod. Phys.* **45**, 44.
BARRETT, R. F., ROBSON, B. A. AND TOBOCMAN, W., 1983, *Rev. Mod. Phys.* **55**, 155.
BATES, D. R. AND SEATON, M. J., 1949, *Mon. Not. R. Astr. Soc.* **109**, 698.
BEDERSON, B., 1969, *Comm. Atom. Molec. Phys.* **1**, 41.
BERGER, R. O. AND SPRUCH, L., 1965, *Phys. Rev.* **138**, B1106.
BETHE, H. A., 1949, *Phys. Rev.* **76**, 38.
BJORKEN, J. D. AND DRELL, S. D., 1964, *Relativistic Quantum Mechanics* (McGraw-Hill, New York).
BLATT, J. M. AND JACKSON, J. D., 1949, *Phys. Rev.* **76**, 18.
BLOCH, C., 1957, *Nucl. Phys.* **4**, 503.
BLUM, K., 1981, *Density Matrix Theory and Applications* (Plenum, New York).
BOTTINO, A., LONGONI, A. M. AND REGGE, T., 1962, *Nuovo Cimento* **23**, 954.
BREIT, G., 1959, *Handbuch der Physik* (Springer, Berlin), **41**, Part 1, n° 1.
BREIT, G. AND WIGNER, E. P., 1936, *Phys. Rev.* **49**, 519.
BRENIG, W. AND HAAG, R., 1959, *Fortschr. Phys.* **7**, 183.
BRILLOUIN, L., 1926, *Comptes Rendus* **183**, 24.
BROWNSTEIN, K. R. AND MCKINLEY, W. A., 1968, *Phys. Rev.* **170**, 1255.
BUCKINGHAM, R. A., 1937, *Proc. Roy. Soc. (London) A* **160**, 94.
BUNYAN, P. J. AND SCHONFELDER, J. L., 1965, *Proc. Phys. Soc.* **85**, 455.
BURGESS, A., 1963, *Proc. Phys. Soc.* **81**, 442.
BURKE, P. G., 1968, *Adv. Atom. Molec. Phys.* **4**, 173.
BURKE, P. G., 1970, *Comput. Phys. Commun.* **1**, 241.
BURKE, P. G., 1977, *Potential Scattering in Atomic Physics* (Plenum, New York).
BURKE, P. G., AND BERRINGTON, K. A., 1993, *Atomic and Molecular Processes: An R-matrix Approach*, (IOP Publishing, Bristol and Philadelphia).
BURKE, P. G., HIBBERT, A. AND ROBB, W. D., 1971, *J. Phys. B* **4**, 153.

BURKE, P. G. AND ROBB, W. D., 1972, *J. Phys. B* **5**, 44.
BURKE, P. G. AND ROBB, W. D., 1975, *Adv. Atom. Molec. Phys.* **11**, 143.
BURKE, P. G., MACKEY, I. AND SHIMAMURA, I., 1977, *J. Phys. B* **10**, 2497.
BUTTLE, P. J. A., 1967, *Phys. Rev.* **160**, 719.
BYRON, F. W., JR. AND JOACHAIN, C. J., 1973a, *Physica* **66**, 33.
BYRON, F. W., JR. AND JOACHAIN, C. J., 1973b, *Phys. Rev. A* **8**, 1267.
BYRON, F. W., JR. AND JOACHAIN, C. J., 1974, *J. Phys. B* **7**, L212.
BYRON, F. W., JR. AND JOACHAIN, C. J., 1977, *Phys. Rep.* **34** C, 233.
BYRON, F. W., JR., JOACHAIN, C. J. AND MUND, E. H., 1973, *Phys. Rev. D* **8**, 2622.
BYRON, F. W., JR., JOACHAIN, C. J. AND MUND, E. H., 1975, *Phys. Rev. D* **11**, 1662.
BYRON, F. W., JR., JOACHAIN, C. J. AND MUND, E. H., 1979, *Phys. Rev. C* **20**, 2325.
BYRON, F. W., JR., JOACHAIN, C. J. AND POTVLIEGE, R. M., 1985, *J. Phys. B* **18**, 1637.
CALLAWAY, J., 1978, *Phys. Rep.* **45**, 89.
CALLAWAY, J., 1980, *Phys. Lett.* **77** A, 137.
CALOGERO, F., 1967 *Variable Phase Approach to Potential Scattering* (Academic Press, New York).
CHATWIN, R. A. AND PURCELL, J. E., 1971, *J. Math. Phys.* **12**, 2024.
CONDON, E. U. AND SHORTLEY, G. H., 1935, *The Theory of Atomic Spectra* (Cambridge University Press).
DALITZ, R. H., 1951, *Proc. Roy. Soc. A* **206**, 509.
DANOS, M. AND GREINER, W., 1966, *Phys. Rev.* **146**, 708.
DARWIN, C. G., 1928, *Proc. Roy. Soc. (London) A* **118**, 654.
DEMKOV, YU. N., 1963, *Variational Principles in the Theory of Collisions* (Pergamon, London).
DEMKOV, YU. N. AND SHEPELENKO, F. P., 1958, *Sov. Phys. JETP* **6**, 1144.
EDMONDS, A. R., 1957, *Angular Momentum in Quantum Mechanics* (Princeton University Press).
FANO, U., 1957, *Rev. Mod. Phys.* **29**, 74.
FANO, U., 1961, *Phys. Rev.* **124**, 1866.
FANO, U. AND LEE, C. M., 1973, *Phys. Rev. Letters* **31**, 1573.
FAXÉN, H. AND HOLTSMARK, J., 1927, *Z. f. Physik* **45**, 307.
FEENBERG, E., 1932, *Phys. Rev.* **40**, 40.
FEYNMAN, R. P., 1949, *Phys. Rev.* **76**, 769.
GAILITIS, M., 1963, *Soviet Physics JETP* **17**, 1328.
GAMOW, G., 1928, *Z. f. Physik* **51**, 204.
GLAUBER, R. J., 1953, *Phys. Rev.* **91**, 459.
GLAUBER, R. J., 1959, in: *Lectures in Theoretical Physics*, W. E. Brittin and L. G. Dunham, eds. (Interscience, New York), Vol. **1**, p. 315.
GOLDBERGER, M. L. AND WATSON, K. M., 1964, *Collision Theory* (Wiley, New York).
GORDON, W., 1928, *Z. f. Physik* **48**, 180.
GREENE, C. H., 1983, *Phys. Rev.* **A28**, 2209.
GREENE, C. H., 1985, *Phys. Rev.* **A32**, 1880.
HAM, F. S., 1955, *Solid St. Phys.* **1**, 217.
HARRIS, F. E., 1967, *Phys. Rev. Letters* **19**, 173.
HARRIS, F. E. AND MICHELS, H. H., 1969, *Phys. Rev. Letters* **22**, 1036.
HARRIS, F. E. AND MICHELS, H. H., 1971, *Meth. Comput. Phys.* **10**, 143.
HARTREE, D. R., 1928, *Proc. Camb. Phil. Soc.* **24**, 426.

HAZI, A. U. AND TAYLOR, H. S., 1970, *Phys. Rev. A* **1**, 1109.
HULTHÉN, L., 1944, *Kgl. Fysiogr. Sallsk. Lund Förh.* **14** (21).
HULTHÉN, L., 1948, *Arkiv. Mat. Ast. Fys.* **35** A, 25.
HYLLERAAS, E. A. AND UNDHEIM, B., 1930, *Z. Phys.* **65**, 759.
JACKSON, J. L., 1951, *Phys. Rev.* **83**, 301.
JEFFREYS, H., 1923, *Proc. Lond. Math. Soc.* (2) **23**, 428.
JOACHAIN, C. J., 1968, in: *Symposia on Theoretical Physics and Mathematics*, A. Ramakrishnan, ed. (Plenum, New York), Vol. **8**, p. 61.
JOACHAIN, C. J., 1983, *Quantum Collision Theory* (North Holland, Amsterdam, 3rd ed.).
JOST, R., 1947, *Helv. Phys. Acta* **20**, 256.
JOST, R. AND PAIS, A., 1951, *Phys. Rev.* **82**, 840.
JOST, K. AND KESSLER, J., 1966, *Z. Phys.* **195**, 1.
KATO, T., 1951, *Progr. Theor. Phys.* **6**, 295, 394.
KEMBLE, E. C., 1937, *The Fundamental Principles of Quantum Mechanics* (McGraw-Hill, New York), Section 21.
KESSLER, J., 1985, *Polarized Electrons* (Springer, Berlin, 2nd ed.).
KLEIN, A. AND ZEMACH, C., 1959, *Ann. Phys. (N. Y.)* **7**, 440.
KOHN, W., 1948, *Phys. Rev.* **74**, 1763.
KOHN, W., 1954, *Rev. Mod. Phys.* **26**, 292.
KRAMERS, H. A., 1926, *Z. Phys.* **39**, 828.
LANDAU, L. D. AND LIFSHITZ, E. M., 1959, *Quantum Mechanics* (Addison–Wesley, Reading, Mass.), Chapter 7.
LANE, A. M. AND ROBSON, D., 1969a, *Phys. Rev.* **178**, 1715.
LANE, A. M. AND ROBSON, D., 1969b, *Phys. Rev.* **185**, 1403.
LANE, A. M. AND THOMAS, R. G., 1958, *Rev. Mod. Phys.* **30**, 257.
LANGER, R. E., 1937, *Phys. Rev.* **51**, 669.
LEE, C. M., 1974, *Phys. Rev. A* **10**, 584.
LE ROUZO, H. AND RASEEV, G., 1984, *Phys. Rev. A* **29**, 1214.
LEVINSON, N., 1949, *K. Dan. Vidensk. Selsk. Mat.-Fys. Medd.* **25**, 9.
LEVY, B. R. AND KELLER, J. B., 1963, *J. Math. Phys.* **4**, 54.
LEWIS, JR., R. R., 1956, *Phys. Rev.* **102**, 537.
LIGHT, J. C. AND WALKER, R. B., 1976, *J. Chem. Phys.* **65**, 4272.
LIGHT, J. C., WALKER, R. B., STECHAL, E. B. AND SCHMALZ, T. G., 1979, *Comput. Phys. Commun.* **17**, 89.
LIPPMANN, B. A. AND SCHWINGER, J., 1950, *Phys. Rev.* **79**, 459.
LIPPMANN, B. A. AND SCHEY, H. M., 1961, *Phys. Rev.* **121**, 1112.
LUCCHESE, R. R., WATSON, D. K. AND MCKOY, V., 1980, *Phys. Rev. A* **22**, 421.
MALIK, F. B., 1962, *Ann. Phys. (N. Y.)* **20**, 464.
MALIK, F. B., 1963, *Ann. Phys. (N. Y.)* **21**, 1.
MESSIAH, A., 1968, *Quantum Mechanics* (Wiley, New York), Vol. 1.
MILLER, W. H. AND JANSEN OP DE HAAR, B. M. D. D., 1987, *J. Chem. Phys.* **86**, 6213.
MILLER, W. H., 1988, *Comm. Atom. Molec. Phys.* **22**, 115.
MOISEIWITSCH, B. L., 1966, *Variational Principles* (Wiley-Interscience, New York).
MOLIÈRE, G., 1947, *Z. Naturforsch* **2** A, 133.
MORGAN, L. A., 1984, *Comput. Phys. Commun.* **31**, 419.
MOTT, N. F., 1929, *Proc. Roy. Soc. (London) A* **124**, 425.

MOTT, N. F. AND MASSEY, H. S. W., 1965, *The Theory of Atomic Collisions* (Oxford University Press, 3rd ed.).
NESBET, R. K., 1968, *Phys. Rev.* **175**, 134.
NESBET, R. K., 1969, *Phys. Rev.* **179**, 60.
NESBET, R. K., 1978, *Phys. Rev. A* **18**, 955.
NESBET, R. K., 1980, *Variational Methods in Electron–Atom Scattering Theory* (Plenum, New York).
NESBET, R. K., 1981a, *J. Phys. B* **14**, L415.
NESBET, R. K., 1981b, *Phys. Rev. A* **24**, 2975.
NESBET, R. K. AND OBEROI, R. S., 1972, *Phys. Rev. A* **6**, 1855.
NOBLE, C. J., BURKE, P. G. AND SALVINI, S., 1982, *J. Phys. B* **15**, 3779.
NORCROSS, D. W. AND SEATON, M. J., 1969, *J. Phys. B* **2**, 731.
NORDHOLM, S. AND BACSKAY, G., 1978, *J. Phys. B* **11**, 193.
NUSSENZVEIG, H. M., 1959, *Nucl. Phys.* **11**, 499.
NUTTALL, J., 1969, *Ann. Phys. (N. Y.)* **52**, 428.
OBEROI, R. S. AND NESBET, R. K., 1973a, *Phys. Rev. A* **8**, 215.
OBEROI, R. S. AND NESBET, R. K., 1973b, *J. Comput. Phys.* **12**, 526.
OBEROI, R. S. AND NESBET, R. K., 1974, *Phys. Rev. A* **9**, 2804.
O'MALLEY, T. F., 1963, *Phys. Rev.* **130**, 1020.
O'MALLEY, T. F., SPRUCH, L. AND ROSENBERG, L., 1961, *J. Math. Phys.* **2**, 491.
O'MALLEY, T. F., BURKE, P. G. AND BERRINGTON, K. A., 1979, *J. Phys. B* **12**, 953.
O'MAHONY, P. F. AND GREENE, C. H., 1985, *Phys. Rev.* **A31**, 250.
PERCIVAL, I. C., 1957, *Proc. Phys. Soc.* **70**, 494.
PERCIVAL, I. C., 1960, *Phys. Rev.* **119**, 159.
PHILPOTT, R. J. AND GEORGE, J., 1974, *Nucl. Phys. A* **233**, 164.
POINCARÉ, H., 1884, *Acta. Math.* **4**, 201.
POTVLIEGE, R. M., 1985, *Thèse de Doctorat* (Université Libre de Bruxelles).
PURCELL, J. E., 1969, *Phys. Rev.* **185**, 1279.
RACAH, G., 1942, *Phys. Rev.* **62**, 438.
RACAH, G., 1943, *Phys. Rev.* **63**, 367.
RAYLEIGH, LORD, 1873, *The Theory of Sound* (reprinted by Dover, New York).
REGGE, T., 1959, *Nuovo Cimento* **14**, 951.
REGGE, T., 1960, *Nuovo Cimento* **18**, 947.
ROSE, M. E., 1957, *Elementary Theory of Angular Momentum* (Wiley, New York).
ROSENBERG, L., SPRUCH, L. AND O'MALLEY, T. F., 1960, *Phys. Rev.* **118**, 184.
RUBINOW, S. I., 1955, *Phys. Rev.* **98**, 183.
RUDGE, M. R. H., 1973, *J. Phys. B* **6**, 1788.
RUDGE, M. R. H., 1975, *J. Phys. B* **8**, 940.
RUDGE, M. R. H., 1990, *J. Phys. B* **23**, 4275.
RUDKJÖBING, M., 1941, *Publ. Kbn. Obs.* **18**, 1.
RUTHERFORD, E., 1911, *Phil. Mag.* **21**, 669.
SCHLESSINGER, L. AND PAYNE, G. L., 1974, *Phys. Rev. A* **10**, 1559.
SCHNEIDER, B. I., 1975a, *Chem. Phys. Letters* **31**, 237.
SCHNEIDER, B. I., 1975b, *Phys. Rev. A* **11**, 1957.
SCHNEIDER, B. I., 1977, in: *The Physics of Electronic and Atomic Collisions*, G. Watel, ed. (North Holland, Amsterdam), 257.
SCHNEIDER, B. I. AND WALKER, R. B., 1979, *J. Chem. Phys.* **70**, 2466.

SCHNEIDER, B. I. AND TAYLOR, H. S., 1982, *J. Chem. Phys.* **77**, 379.
SCHONFELDER, J. L., 1966, *Proc. Phys. Soc.* **87**, 163.
SCHWARTZ, C., 1961a, *Phys. Rev.* **124**, 1468.
SCHWARTZ, C., 1961b, *Ann. Phys.* (*N. Y.*) **16**, 36.
SCHWINGER, J., 1947, unpublished lecture notes, (Harvard University), *Phys. Rev.* **72**, 742.
SEATON, M. J., 1955, *Comp. Rend.* **240**, 1317.
SEATON, M. J., 1958, *Mon. Not. R. Astron. Soc.* **118**, 504.
SEATON, M. J., 1966a, *Proc. Phys. Soc.* **88**, 801.
SEATON, M. J., 1966b, *Proc. Phys. Soc.* **88**, 815.
SEATON, M. J., 1983, *Rep. Prog. Phys.* **46**, 167.
SHERMAN, N., 1956, *Phys. Rev.* **103**, 1601.
SHIMAMURA, I., 1977a, *J. Phys. B* **10**, 2597.
SHIMAMURA, I., 1977b, in: *The Physics of Electronic and Atomic Collisions*, G. Watel, ed. (North Holland, Amsterdam), 257.
SIEGERT, A. J. F., 1939, *Phys. Rev.* **56**, 750.
SLOAN, I. H., 1964, *Proc. Roy. Soc.* (*London*) *A* **281**, 151.
SPRUCH, L., 1962, in: *Lectures in Theoretical Physics*, W. E. Brittin, B. W. Downs and J. Downs, eds. (Interscience, New York), Vol. **4**, p. 161.
SPRUCH, L. AND ROSENBERG, L., 1959, *Phys. Rev.* **116**, 1034.
SUGAR, R. AND BLANKENBECLER, R., 1964, *Phys. Rev. B* **136**, 472.
SWIFT, A., 1974, *Phys. Rev. D* **9**, 1740.
TAKATSUKA, K., LUCCHESE, R. R. AND MCKOY, V., 1981, *Phys. Rev. A* **24**, 18'12.
TAMM, I. G., 1944, *Sh. Eksper. i. Teor. Fiz.* **14**, 21.
TAMM, I. G., 1948, *Sh. Eksper. i. Teor. Fiz.* **18**, 337.
TAMM, I. G., 1949, *Sh. Eksper. i. Teor. Fiz.* **19**, 74.
TEMKIN, A., 1966, in: *Autoionization*, ed. A. Temkin (Mono Book Corp., Baltimore), 55.
TEMPLE, G., 1928, *Proc. Roy. Soc.* (*London*) *A* **121**, 673.
TER HAAR, D., 1961, *Rep. Progr. Phys.* **24**, 304.
THIRUMALAI, D. AND TRUHLAR, D. G., 1980, *Chem. Phys. Letters* **70**, 330.
TOBOCMAN, W. AND NAGARAJAN, M. A., 1965a, *Phys. Rev.* **138**, B1351.
TOBOCMAN, W. AND NAGARAJAN, M. A., 1965b, *Phys. Rev.* **140**, B63.
VON NEUMANN, J., 1927, *Nachr. Deut. Akad. Wiss. G"ottingen, Math. -Phys. Kl.*, 245 and 273.
WALKER, D. W., 1971, *Adv. Phys.* **20**, 257.
WALLACE, S. J., 1973a, *Ann. Phys.* (*N. Y.*) **78**, 190.
WALLACE, S. J., 1973b, *Phys. Rev. D* **8**, 1846, 1934.
WATSON, G. N., 1966, *A Treatise on the Theory of Bessel Functions* (Cambridge University Press, 2nd ed.).
WATSON, D. K., LUCCHESE, R. R. AND MCKOY, V., 1980, *Phys. Rev. A* **21**, 738.
WENTZEL, G., 1926, *Z. f. Physik* **38**, 518.
WHITTAKER, E. T. AND WATSON, G. N., 1935, *A Course of Modern Analysis* (Cambridge University Press, 4th ed.), 337.
WIGNER, E. P., 1940, unpublished paper reproduced in: *Quantum Theory of Angular Momentum* L. C. Biedenharn and H. Van Dam, eds., (Academic Press, New York, 1965) p. 89.
WIGNER, E. P., 1946a, *Phys. Rev.* **70**, 15.

WIGNER, E. P., 1946b, *Phys. Rev.* **70**, 606.
WIGNER, E. P., 1955, *Phys. Rev.* **98**, 145.
WIGNER, E. P. AND EISENBUD, L., 1947, *Phys. Rev.* **72**, 29.
WLADAWSKI, I., 1973, *J. Chem. Phys.* **58**, 1826.
WÜBKER, W., MÖLLENKAMP, R. AND KESSLER, J., 1982, *Phys. Rev. Lett.* **49**, 272.
YOST, F. L., WHEELER, J. AND BREIT, G., 1936, *Phys. Rev.* **49**, 174.
ZEMACH, C. AND KLEIN, A., 1958, *Nuovo Cimento* **10**, 1078.
ZHANG, J. Z. H., CHU, S. -I. AND MILLER, W. H., 1988, *J. Chem. Phys.* **88**, 6233.
ZVIJAC, D. J., HELLER, J. AND LIGHT, J. C., 1975, *J. Phys. B* **8**, 1016.

INDEX