Chapter 7

Motion in Spherically Symmetric Potentials

We describe in this section the stationary bound states of quantum mechanical particles in spherically symmetric potentials $V(r)$, i.e., in potentials which are solely a function of r and are independent of the angles θ, ϕ. Four examples will be studied. The first potential

$$V(r) \; = \; \begin{cases} 0 & 0 \leq r \leq R \\ \infty & r > R \end{cases} \tag{7.1}$$

confines a freely moving particle to a spherical box of radius R. The second potential is of the square well type

$$V(r) \; = \; \begin{cases} -V_o & 0 \leq r \leq R \\ 0 & r > R \end{cases} \; . \tag{7.2}$$

The third potential

$$V(r) \; = \; \frac{1}{2} m \omega^2 r^2 \tag{7.3}$$

describes an isotropic harmonic oscillator . The fourth potential

$$V(r) \; = \; - \frac{Z\, e^2}{r} \tag{7.4}$$

governs the motion of electrons in hydrogen-type atoms.

Potential (7.4) is by far the most relevant of the four choices. It leads to the stationary electronic states of the hydrogen atom ($Z = 1$). The corresponding wave functions serve basis functions for multi-electron systems in atoms, molecules, and crystals. The potential (7.3) describes the motion of a charge in a uniformely charged sphere and can be employed to describe the motion of protons and neutrons in atomic nuclei[1]. The potentials (7.1, 7.2) serve as schematic descriptions of quantum particles, for example, in case of the so-called bag model of hadronic matter.

[1]See, for example, *Simple Models of Complex Nuclei / The Shell Model and the Interacting Boson Model* by I. Talmi (Harwood Academic Publishers, Poststrasse 22, 7000 Chur, Switzerland, 1993)

7.1 Radial Schrödinger Equation

A classical particle moving in a potential $V(r)$ is governed by the Newtonian equation of motion

$$m\dot{\vec{v}} \;=\; -\,\hat{e}_r\,\partial_r V(r)\;. \tag{7.5}$$

In the case of an angular independent potential angular momentum $\vec{J} = m\,\vec{r}\times\vec{v}$ is a constant of motion. In fact, the time variation of $\vec{J}$ can be written, using (7.5) and $\dot{\vec{r}} = \vec{v}$,

$$\frac{d}{dt}\vec{J} \;=\; \vec{v}\times m\vec{v} \;+\; \vec{r}\times m\dot{\vec{v}} \;=\; 0 \;+\; \vec{r}\times\hat{e}_r\,(-\partial_r V(r)) \;=\; 0\;. \tag{7.6}$$

Since $\dot{J}_k$ is also equal to the poisson bracket $\{H, J_k\}$ where H is the Hamiltonian, one can conclude

$$\dot{J}_k \;=\; \{H, J_k\} \;=\; 0\,,\quad k \;=\; 1,2,3. \tag{7.7}$$

The correspondence principle dictates then for the quantum mechanical Hamiltonian operator $\hat{H}$ and angular momentum operators $\mathcal{J}_k$

$$[\hat{H},\,\mathcal{J}_k] \;=\; 0\,,\quad k \;=\; 1,2,3\;. \tag{7.8}$$

This property can also be proven readily employing the expression of the kinetic energy operator [c.f. (5.99)]

$$-\frac{\hbar^2}{2m}\nabla^2 \;=\; -\frac{\hbar^2}{2m}\,\frac{1}{r}\,\partial_r^2\,r \;+\; \frac{\mathcal{J}^2}{2mr^2}\;, \tag{7.9}$$

the expressions (5.85– 5.87) for $\mathcal{J}_k$ as well as the commutation property (5.61) of $\mathcal{J}^2$ and $\mathcal{J}_k$. Accordingly, stationary states $\psi_{E,\ell,m}(\vec{r})$ can be chosen as simultaneous eigenstates of the Hamiltonian operator $\hat{H}$ as well as of $\mathcal{J}^2$ and $\mathcal{J}_3$, i.e.,

$$\hat{H}\,\psi_{E,\ell,m}(\vec{r}) \;=\; E\,\psi_{E,\ell,m}(\vec{r}) \tag{7.10}$$

$$\mathcal{J}^2\psi_{E,\ell,m}(\vec{r}) \;=\; \hbar^2\ell(\ell+1)\,\psi_{E,\ell,m}(\vec{r}) \tag{7.11}$$

$$\mathcal{J}_3\psi_{E,\ell,m}(\vec{r}) \;=\; \hbar\,m\,\psi_{E,\ell,m}(\vec{r})\;. \tag{7.12}$$

In classical mechanics one can exploit the conservation of angular momentum to reduce the equation of motion to an equation governing solely the radial coordinate of the particle. For this purpose one concludes first that the conservation of angular momentum $\vec{J}$ implies a motion of the particle confined to a plane. Employing in this plane the coordinates r, θ for the distance from the origin and for the angular position, one can state

$$J \;=\; m\,r^2\,\dot{\theta}\;. \tag{7.13}$$

The expression of the kinetic energy

$$\frac{\vec{p}^2}{2m} \;=\; \frac{1}{2}m\,\dot{r}^2 \;+\; \frac{1}{2}m\,r^2\dot{\theta}^2 \;=\; \frac{1}{2}m\,\dot{r}^2 \;+\; \frac{J^2}{2mr^2} \tag{7.14}$$

and conservation of energy yield

$$\frac{1}{2}m\,\dot{r}^2 \;+\; \frac{J^2}{2mr^2} \;+\; V(r) \;=\; E\;. \tag{7.15}$$

This is a differential equation which governs solely the radial coordinate. It can be solved by integration of

$$\dot{r} \;=\; \pm \left\{ \frac{2}{m} \left[E \,-\, V(r) \,-\, \frac{J^2}{2mr^2} \right] \right\}^{\frac{1}{2}} \;. \tag{7.16}$$

Once, $r(t)$ is determined the angular motion follows from (7.13), i.e., by integration of

$$\dot{\theta} \;=\; \frac{J}{mr^2(t)} \;. \tag{7.17}$$

In analogy to the classical description one can derivem, in the present case, for the wave function of a quantum mechanical particle a differential equation which governs solely the r-dependence. Employing the kinetic energy operator in the form (7.9) one can write the stationary Schrödinger equation (7.10), using (7.11),

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r} \partial_r^2 \, r \,+\, \frac{\mathcal{J}^2}{2mr^2} \,+\, V(r) \,-\, E_{\ell,m} \right] \psi_{E,\ell,m}(\vec{r}) \;=\; 0 \;. \tag{7.18}$$

Adopting for $\psi_{E,\ell,m}(\vec{r})$ the functional form

$$\psi_{E,\ell,m}(\vec{r}) \;=\; v_{E,\ell,m}(r)\, Y_{\ell m}(\theta,\phi) \tag{7.19}$$

where $Y_{\ell m}(\theta,\phi)$ are the angular momentum eigenstates defined in Section 5.4, equations (7.11, 7.12) are obeyed and one obtains for (7.10)

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r} \partial_r^2 \, r \,+\, \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \,+\, V(r) \,-\, E_{\ell,m} \right] v_{E,\ell,m}(r) \;=\; 0 \;. \tag{7.20}$$

Since this equation is independent of the quantum number m we drop the index m on the radial wave function $v_{E,\ell,m}(r)$ and $E_{\ell,m}$.

One can write (7.20) in the form of the one-dimensional Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \partial_r^2 \,+\, V_{\text{eff}}(r) \,-\, E \right] \phi_E(r) \;=\; 0 \;. \tag{7.21}$$

where

$$V_{\text{eff}}(r) \;=\; V(r) \,+\, \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \tag{7.22}$$

$$\phi_E(r) \;=\; r\, v_{E,\ell,m}(r) \;. \tag{7.23}$$

This demonstrates that the function $r\, v_{E,\ell,m}(r)$ describes the radial motion as a one-dimensional motion in the interval $[0, \infty[$ governed by the effective potential (7.22) which is the original potential $V(r)$ with an added rotational barrier potential $\frac{\hbar^2 \ell(\ell+1)}{2mr^2}$. This barrier, together with the original potential, can exclude particles from the space with small r values, but can also trap particles in the latter space giving rise to strong scattering resonances (see Section **??**).

Multiplying (7.20) by $-2mr/\hbar^2$ yields the so-called *radial Schrödinger equation*

$$\left[\partial_r^2 \,-\, \frac{\ell(\ell+1)}{r^2} \,-\, U(r) \,-\, \kappa_\ell^2 \right] r\, v_{\kappa,\ell}(r) \;=\; 0 \;. \tag{7.24}$$

where we defined

$$U(r) = -\frac{2m}{\hbar^2} V(r) \tag{7.25}$$

$$\kappa_\ell^2 = -\frac{2m}{\hbar^2} E_\ell \tag{7.26}$$

In case $E < 0$, κ assumes real values. We replaced in (7.20) the index E by the equivalent index κ.

Boundary Conditions

In order to solve (7.20) one needs to specify proper boundary conditions[2]. For $r \to 0$ one may assume that the term $\ell(\ell+1)/r^2$ becomes larger than the potential $U(r)$. In this case the solution is governed my

$$\left[\partial_r^2 - \frac{\ell(\ell+1)}{r^2} \right] r\, v_{\kappa,\ell}(r) = 0 \,, \quad r \to 0 \tag{7.27}$$

and, accordingly, assumes the general form

$$r\, v_{\kappa,\ell}(r) \sim A\, r^{\ell+1} + B\, r^{-\ell} \tag{7.28}$$

or

$$v_{\kappa,\ell}(r) \sim A\, r^{\ell} + B\, r^{-\ell-1} \tag{7.29}$$

Only the first term is admissable. This follows for $\ell > 0$ from consideration of the integral which measures the total particle density. The radial part of this integral is

$$\int_0^\infty dr\, r^2\, v_{\kappa,\ell}^2(r) \tag{7.30}$$

and, hence, the term $Br^{-(\ell+1)}$ would contribute

$$|B|^2 \int_0^\epsilon dr\, r^{-2\ell} \tag{7.31}$$

which, for $\ell > 0$ is not integrable. For $\ell = 0$ the contribution of $Br^{-(\ell+1)}$ to the complete wave function is, using the expression (5.182) for Y_{00},

$$\psi_{E,\ell,m}(\vec{r}) \sim \frac{B}{\sqrt{4\pi}|\vec{r}|} \,. \tag{7.32}$$

The total kinetic energy resulting from this contribution is, according to a well-known result in *Classical Electromagnetism*[3],

$$\frac{\hbar^2}{2m} \nabla^2 \psi_{E,\ell,m}(\vec{r}) \sim \sqrt{4\pi}\, B\, \delta(x_1)\delta(x_2)\delta(x_3) \,. \tag{7.33}$$

[2]A detailed discussion of the proper boundary conditions, in particular, at $r = 0$ is found in the excellent monographs *Quantum Mechanics I, II* by A. Galindo and P. Pascual (Springer, Berlin, 1990)

[3]We refer here to the fact that the function $\Phi(\vec{r}) = 1/r$ is the solution of the Poisson equation $\nabla^2 = -4\pi\delta(x)\delta(y)\delta(z)$; see, for example, "Classical Electrodynamics, 2nd Ed." by J.D. Jackson (John Wiley, New York, 1975).

Since there is no term in the stationary Schrödinger equation which could compensate this δ-function contribution we need to postulate that the second term in (7.29) is not permissible. One can conclude that the solution of the radial Schrödinger equation must obey

$$r\, v_{\kappa,\ell}(r) \;\to\; 0 \quad \text{for } r \;\to\; 0\;. \tag{7.34}$$

The boundary conditions for $r \to \infty$ are governed by two terms in the radial Schrödinger equation, namely,

$$\left[\,\partial_r^2 \;-\; \kappa_\ell^2\,\right] r\, v_{\kappa,\ell}(r) \;=\; 0 \quad \text{for } r \;\to\; \infty \;\;. \tag{7.35}$$

We have assumed here $\lim_{r\to\infty} V(r) \;=\; 0$ which is the convention for potentials. The solution of this equation is

$$r\, v_{\kappa,\ell}(r) \;\sim\; A\, e^{-\kappa r} \;+\; B\, e^{+\kappa r} \quad \text{for } r \;\to\; \infty\;. \tag{7.36}$$

For bound states κ is real and, hence, the second contribution is not permissible. We conclude, therefore, that the asymptotic boundary condition for the solution of the radial Schrödinger equation (7.20) is

$$r\, v_{\kappa,\ell}(r) \;\sim\; e^{-\kappa r} \quad \text{for } r \;\to\; \infty\;. \tag{7.37}$$

Degeneracy of Energy Eigenvalues

We have noted above that the differential operator appearing on the l.h.s. of the in radial Schrödinger equation (7.24) is independent of the angular momentum quantum number m. This implies that the energy eigenvalues associated with stationary bound states of radially symmetric potentials with identical ℓ, but different m quantum number, assume the same values. This behaviour is associated with the fact that any rotational transformation of a stationary state leaves the energy of a stationary state unaltered. This property holds since (7.8) implies

$$[\hat{H},\, \exp(-\frac{i}{\hbar}\vartheta\cdot\vec{\mathcal{J}})\,] \;=\; 0\;. \tag{7.38}$$

Applying the rotational transformation $\exp(-\frac{i}{\hbar}\vartheta\cdot\vec{\mathcal{J}})$ to (7.10) yields then

$$\hat{H}\; \exp(-\frac{i}{\hbar}\vartheta\cdot\vec{\mathcal{J}})\, \psi_{E,\ell,m}(\vec{r}) \;=\; E\; \exp(-\frac{i}{\hbar}\vartheta\cdot\vec{\mathcal{J}})\, \psi_{E,\ell,m}(\vec{r})\;, \tag{7.39}$$

i.e., any rotational transformation produces energetically degenerate stationary states. One might also apply the operators $\mathcal{J}_\pm \;=\; \mathcal{J}_1 \,\pm\, i\mathcal{J}_2$ to (7.10) and obtain for $-\ell \,<\, m \,<\, \ell$

$$\hat{H}\, \mathcal{J}_\pm\, \psi_{E,\ell,m}(\vec{r}) \;=\; E\, \mathcal{J}_\pm\, \psi_{E,\ell,m}(\vec{r})\;, \tag{7.40}$$

which, together with the identities (5.172, 5.173), yields

$$\hat{H}\, \psi_{E,\ell,m\pm 1}(\vec{r}) \;=\; E\, \psi_{E,\ell,m\pm 1}(\vec{r}) \tag{7.41}$$

where E is the same eigenvalue as in (7.40). One expect, therefore, that the stationary states for spherically symmetric potentials form groups of $2\ell + 1$ energetically degenerate states, so-called multiplets where $\ell \;=\; 0, 1, 2, \ldots$. Following a convention from atomic spectroscopy, one refers to the multiplets with $\ell \;=\; 0, 1, 2, 3$ as the s, p, d, f-multipltes, respectively.

In the remainder of this section we will solve the radial Schrödinger equation (7.20) for the potentials stated in (7.1–7.4). We seek to describe bound states for the particles, i.e., states with $E \,<\, 0$. States with $E \,>\, 0$, which play a key role in scattering processes, will be described in Section **??**.

7.2 Free Particle Described in Spherical Coordinates

We consider first the case of a particle moving in a force-free space described by the potential

$$V(r) \equiv 0 . \tag{7.42}$$

The stationary Schrödinger equation for this potential reads

$$\left[-\frac{\hbar^2}{2m} \nabla^2 - E \right] \psi_E(\vec{r}) = 0 . \tag{7.43}$$

Stationary States Expressed in Cartesian Coordinates The general solution of (7.43), as expressed in (3.74–3.77), is

$$\psi(\vec{k}|\vec{r}) = N e^{i\vec{k}\cdot\vec{r}} \tag{7.44}$$

where

$$E = \frac{\hbar^2 k^2}{2m} \geq 0 . \tag{7.45}$$

The possible energies can assume continuous values. N in (7.44) is some suitably chosen normalization constant; the reader should be aware that (7.44) does not represent a localized particle and that the function is not square integrable. One chooses N such that the orthonormality property

$$\int_{\Omega_\infty} d^3r \; \psi^*(\vec{k}'|\vec{r})\psi(\vec{k}|\vec{r}) = \delta(\vec{k}' - \vec{k}) \tag{7.46}$$

holds. The proper normalization constant is $N = (2\pi)^{-3/2}$.
In case of a force-free motion momentum is conserved. In fact, the Hamiltonian in the present case

$$H_o = -\frac{\hbar^2}{2m} \nabla^2 \tag{7.47}$$

commutes with the momentum operator $\hat{\vec{p}} = (\hbar/i)\nabla$ and, accordingly, the eigenfunctions of (7.45) can be chosen as simultaneous eigenfunction of the momentum operator. In fact, it holds

$$\hat{\vec{p}} N e^{i\vec{k}\cdot\vec{r}} = \hbar\vec{k} \, N e^{i\vec{k}\cdot\vec{r}} . \tag{7.48}$$

as one can derive using in (7.48) Cartesian coordinates, i.e.,

$$\nabla = \begin{pmatrix} \partial_1 \\ \partial_2 \\ \partial_3 \end{pmatrix} , \quad \vec{k}\cdot\vec{r} = k_1x_1 + k_2x_2 + k_3x_3 . \tag{7.49}$$

Stationary States Expressed in Spherical Coordinates Rather than specifying energy through $k = |\vec{k}|$ and the direction of the momentum through $\hat{k} = \vec{k}/|\vec{k}|$ one can exploit the fact that the angular momentum operators $\mathcal{J}^2$ and $\mathcal{J}_3$ given in (5.97) and in (5.92), respectively, commute with H_o as defined in (7.47). This latter property follows from (5.100) and (5.61). Accordingly, one can choose stationary states of the free particle which are eigenfunctions of (7.47) as well as eigenfunctions of $\mathcal{J}^2$ and $\mathcal{J}_3$ described in Sect. 5.4.

The corresponding stationary states, i.e., solutions of (7.43) are given by wave functions of the form

$$\psi(k,\ell,m|\vec{r}) \;=\; v_{k,\ell}(r)\, Y_{\ell m}(\theta,\phi) \tag{7.50}$$

where the radial wave functions obeys [c.f. (7.20)]

$$\left[-\frac{\hbar^2}{2m}\,\frac{1}{r}\,\partial_r^2\, r \;+\; \frac{\hbar^2 \ell(\ell+1)}{2mr^2} \;-\; E_{\ell,m} \right] v_{k,\ell}(r) \;=\; 0\,. \tag{7.51}$$

Using (7.45) and multiplying (7.20) by $-2mr/\hbar^2$ yields the radial Schrödinger equation

$$\left[\partial_r^2 \;-\; \frac{\ell(\ell+1)}{r^2} \;+\; k^2 \right] r\, v_{k,\ell}(r) \;=\; 0\,. \tag{7.52}$$

We want to determine now the solutions $v_{k,\ell}(r)$ of this equation.
We first notice that the solution of (7.52) is actually only a function of kr, i.e., one can write $v_{k,\ell}(r) = j_\ell(kr)$. In fact, one can readily show, introducing the new variable $z = kr$, that (7.52) is equivalent to

$$\left[\frac{d^2}{dz^2} \;-\; \frac{\ell(\ell+1)}{z^2} \;+\; 1 \right] z\, j_\ell(z) \;=\; 0\,. \tag{7.53}$$

According to the discussion in Sect. 7.1 the regular solution of this equation, at small r, behaves like

$$j_\ell(z) \;\sim\; z^\ell \quad \text{for} \quad r \to 0\,. \tag{7.54}$$

There exists also a so-called irregular solution of (7.53), denoted by $n_\ell(z)$ which behaves like

$$n_\ell(z) \;\sim\; z^{-\ell-1} \quad \text{for} \quad r \to 0\,. \tag{7.55}$$

We will discuss further below also this solution, which near $r = 0$ is inadmissable in a quantum mechanical wave function, but admissable for $r \neq 0$.
For large z values the solution of (7.53) is governed by

$$\left[\frac{d^2}{dz^2} \;+\; 1 \right] z\, j_\ell(z) \;=\; 0 \quad \text{for} \quad r \to \infty \tag{7.56}$$

the general solution of which is

$$j_\ell(z) \;\sim\; \frac{1}{z}\, \sin(z \,+\, \alpha) \quad \text{for} \quad r \to \infty \tag{7.57}$$

for some phase α.
We note in passing that the functions $g_\ell(z) = j_\ell(z), n_\ell(z)$ obey the differential equation equivalent to (7.53)

$$\left[\frac{d^2}{dz^2} \;+\; \frac{2}{z}\,\frac{d}{dz} \;-\; \frac{\ell(\ell+1)}{z^2} \;+\; 1 \right] g_\ell(z) \;=\; 0\,. \tag{7.58}$$

Noting that $\sin(z + \alpha)$ can be written as an infinite power series in z we attempt to express the solution of (7.53) for arbitary z values in the form

$$j_\ell(z) \;=\; z^\ell\, f(z^2)\,, \quad f(z^2) \;=\; \sum_{n=0}^{\infty} a_n\, z^{2n}\,. \tag{7.59}$$

The unknown expansion coefficients can be obtained by inserting this series into (7.53). We have introduced here the assumption that the factor f in (7.59) depends on z^2. This follows from

$$\frac{d^2}{dz^2} z^{\ell+1} f(z) \;=\; z^{\ell+1} \frac{d^2}{dz^2} f(z) \;+\; 2(\ell+1) z^{\ell} \frac{d}{dz} f \;+\; \ell(\ell+1) z^{\ell-1} f \tag{7.60}$$

from which we can conclude

$$\left(\frac{d^2}{dz^2} \;+\; (\ell+1) \frac{2}{z} \frac{d}{dz} \;+\; 1 \right) f(z) \;=\; 0 \,. \tag{7.61}$$

Introducing the new variable $v \;=\; z_2$ yields, using

$$\frac{1}{z} \frac{d}{dz} \;=\; 2 \frac{d}{dv} \,, \quad \frac{d^2}{dz^2} \;=\; 4v \frac{d^2}{dv^2} \;+\; 2 \frac{d}{dv} \,, \tag{7.62}$$

the differential equation

$$\left(\frac{d^2}{dv^2} \;+\; \frac{2\ell+3}{2v} \frac{d}{dv} \;+\; \frac{1}{4v} \right) f(v) \;=\; 0 \tag{7.63}$$

which is consistent with the functional form in (7.59). The coefficients in the series expansion of $f(z^2)$ can be obtained from inserting $\sum_{n=0}^{\infty} a_n \, z^{2n}$ into (7.63) ($v \;=\; z^2$)

$$\sum_n \left(a_n \, n \, (n-1) \, v^{n-2} \;+\; \frac{1}{2} (2\ell+3) \, a_n \, v^{n-2} \;+\; \frac{1}{4} a_n \, v^{n-1} \right) \;=\; 0 \tag{7.64}$$

Changing the summation indices for the first two terms in the sum yields

$$\sum_n \left(a_{n+1} \, n \, (n-1) \;+\; \frac{1}{2} (2\ell+3) \, a_n \;+\; \frac{1}{4} a_n \right) v^{n-1} \;=\; 0 \,. \tag{7.65}$$

In this expression each term $\sim v^{n-1}$ must vanish individually and, hence,

$$a_{n+1} \;=\; -\frac{1}{2} \frac{1}{(n+1)\,(2n \;+\; 2\ell \;+\; 3)} \, a_n \tag{7.66}$$

One can readily derive

$$a_1 \;=\; -\frac{1}{2} \frac{1}{1!\,(2\ell+3)} \, a_0 \,, \quad a_2 \;=\; \frac{1}{4} \frac{1}{2!\,(2\ell+3)(2\ell+5)} \, a_0 \,. \tag{7.67}$$

The common factor a_0 is arbitrary. Choosing

$$a_0 \;=\; \frac{1}{1 \cdot 3 \cdot 5 \cdot (2\ell+1)} \,. \tag{7.68}$$

the ensuing functions ($\ell \;=\; 0, 1, 2, \ldots$)

$$j_\ell(z) \;=\; \frac{z^\ell}{1 \cdot 3 \cdot 5 \cdots (2\ell+1)} \left[1 \;-\; \frac{\frac{1}{2} z^2}{1!(2\ell+3)} \;+\; \frac{(\frac{1}{2} z^2)^2}{2!(2\ell+3)(2\ell+5)} \;-\; + \;\cdots \right] \tag{7.69}$$

are called *regular spherical Bessel functions*.

One can derive similarly for the solution (7.55) the series expansion ($\ell = 0, 1, 2, \ldots$)

$$n_\ell(z) \;=\; -\frac{1 \cdot 3 \cdot 5 \cdots (2\ell - 1)}{z^{\ell+1}} \left[1 \;-\; \frac{\frac{1}{2}z^2}{1!(1-2\ell)} \;+\; \frac{(\frac{1}{2}z^2)^2}{2!(1-2\ell)(3-2\ell)} \;-+\cdots \right] . \tag{7.70}$$

These functions are called *irregular spherical Bessel functions*.

Exercise 7.2.1: Demonstrate that (7.70) is a solution of (7.52) obeying (7.55).

The Bessel functions (7.69, 7.70) can be expressed through an infinite sum which we want to specify now. For this purpose we write (7.69)

$$\begin{aligned} j_\ell(z) \;&=\; \left(\frac{z}{2}\right)^\ell \frac{1}{\frac{1}{2}\cdot\frac{3}{2}\cdot\frac{5}{2}\cdots(\ell+\frac{1}{2})} \\ &\qquad \left[1 \;+\; \frac{((\frac{iz}{2})^2}{1!(\ell+\frac{3}{2})} \;+\; \frac{(((\frac{iz}{2})^4}{2!(\ell+\frac{3}{2})(2\ell+\frac{5}{2})} \;+\cdots \right] \end{aligned} \tag{7.71}$$

The factorial-type products

$$\frac{1}{2}\cdot\frac{3}{2}\cdots\left(\ell+\frac{1}{2}\right) \tag{7.72}$$

can be expressed through the so-called Gamma-function[4] defined through

$$\Gamma(z) \;=\; \int_0^\infty dt\, t^{z-1}\, e^{-t} \,. \tag{7.73}$$

This function has the following properties[5]

$$\Gamma(z+1) \;=\; z\,\Gamma(z) \tag{7.74}$$
$$\Gamma(n+1) \;=\; n! \quad \text{for } n \in \mathbb{N} \tag{7.75}$$
$$\Gamma(\tfrac{1}{2}) \;=\; \sqrt{\pi} \tag{7.76}$$
$$\Gamma(z)\,\Gamma(1-z) \;=\; \frac{\pi}{\sin \pi z} \,. \tag{7.77}$$

from which one can deduce readily

$$\Gamma(\ell+\tfrac{1}{2}) \;=\; \sqrt{\pi}\cdot\frac{1}{2}\cdot\frac{3}{2}\cdots\left(\ell+\frac{1}{2}\right) \,. \tag{7.78}$$

One can write then

$$j_\ell(z) \;=\; \frac{\sqrt{\pi}}{2}\left(\frac{z}{2}\right)^\ell \sum_{n=0}^{\infty} \frac{\left(\frac{iz}{2}\right)^{2n}}{n!\,\Gamma(n+1+\ell+\frac{1}{2})} \,. \tag{7.79}$$

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[4]For further details see *Handbook of Mathematical Functions* by M. Abramowitz and I.A. Stegun (Dover Publications, New York)

[5]The proof of (7.74–7.76) is elementary; a derivation of (7.77) can be found in *Special Functions of Mathematical Physics* by A.F. Nikiforov and V.B. Uvarov, Birkhäuser, Boston, 1988)

Similarly, one can express $n_\ell(z)$ as given in (7.70)

$$n_\ell(z) \;=\; -\frac{2^\ell}{\sqrt{\pi} z^{\ell+1}}\,\Gamma(\ell+\frac{1}{2})\;\left[1 \,+\, \frac{\left(\frac{iz}{2}\right)^2}{1!(\frac{1}{2}-\ell)} \,+\, \frac{\left(\frac{iz}{2}\right)^4}{2!(\frac{1}{2}-\ell)(\frac{3}{2}-\ell)} \,+\,\cdots\right]. \tag{7.80}$$

Using (7.77) for $z = \ell + \frac{1}{2}$, i.e.,

$$\Gamma(\ell+\tfrac{1}{2}) \;=\; (-1)^\ell\,\frac{\pi}{\Gamma(\frac{1}{2}-\ell)} \tag{7.81}$$

yields

$$\begin{aligned} n_\ell(z) \;&=\; (-1)^{\ell+1}\sqrt{\pi}\,\frac{2^\ell}{z^{\ell+1}}\left[\frac{1}{\Gamma(\frac{1}{2}-\ell)} \,+\, \frac{\left(\frac{iz}{2}\right)^2}{1!\,\Gamma(\frac{1}{2}-\ell)(\frac{1}{2}-\ell)}\right. \\ &\quad \left. +\,\frac{\left(\frac{iz}{2}\right)^4}{2!\,\Gamma(\frac{1}{2}-\ell)(\frac{1}{2}-\ell)(\frac{3}{2}-\ell)} \,+\,\cdots\right]. \end{aligned} \tag{7.82}$$

or

$$n_\ell(z) \;=\; (-1)^{\ell+1}\,\frac{\sqrt{\pi}}{2}\left(\frac{2}{z}\right)^{\ell+1}\sum_{n=0}^{\infty}\frac{\left(\frac{iz}{2}\right)^{2n}}{n!\,\Gamma(n+1-\ell-\frac{1}{2})}\,. \tag{7.83}$$

Linear independence of the Regular and Irregular spherical Bessel Functions

We want to demonstrate now that the solutions (7.69) and (7.69) of (7.53) are linearly independent. For this purpose we need to demonstrate that the Wronskian

$$W(j_\ell, n_\ell) \;=\; j_\ell(z)\,\frac{d}{dz}\,n_\ell \;-\; \frac{d}{dz}\,j_\ell(z)\,n_\ell \tag{7.84}$$

does not vanish. Let f_1, f_2 be solutions of (7.53), or equivalently, of (7.58). Using

$$\frac{d^2}{dz^2}\,f_{1,2} \;=\; -\,\frac{2}{z}\,\frac{d}{dz}\,f_{1,2} \,+\, \frac{\ell(\ell+1)}{z^2}\,f_{1,2} \,-\, f_{1,2} \tag{7.85}$$

one can demonstrate the identity

$$\frac{d}{dz}\,W(f_1,f_2) \;=\; -\frac{2}{z}\,W(f_1,f_2) \tag{7.86}$$

This equation is equivalent to

$$\frac{d}{dz}\ln W \;=\; \frac{d}{dz}\ln\frac{1}{z^2} \tag{7.87}$$

the solution of which is

$$\ln W \;=\; \frac{c}{z^2} \tag{7.88}$$

for some constant c. For the case of $f_1 = j_\ell$ and $f_2 = n_\ell$ this constant can be determined using the expansions (7.69, 7.70) keeping only the leading terms. One obtains $c = 1$ and, hence,

$$W(j_\ell, n_\ell) \;=\; \frac{1}{z^2}\,. \tag{7.89}$$

The Wronskian (7.89) doesn not vanish and, therefore, the regular and irregular Bessel functions are linearly independent.

Relationship to Bessel functions

The differential equation (7.58) for the spherical Bessel functions $g_\ell(z)$ can be simplified by seeking the corresponding equation for $G_{\ell+\frac{1}{2}}(z)$ defined through

$$g_\ell(z) \;=\; \frac{1}{\sqrt{z}}\, G_{\ell+\frac{1}{2}}(z). \tag{7.90}$$

Using

$$\frac{d}{dz}\, g_\ell(z) \;=\; \frac{1}{\sqrt{z}}\,\frac{d}{dz}\, G_{\ell+\frac{1}{2}}(z) \;-\; \frac{1}{2z\sqrt{z}}\, G_{\ell+\frac{1}{2}}(z) \tag{7.91}$$

$$\frac{d^2}{dz^2}\, g_\ell(z) \;=\; \frac{1}{\sqrt{z}}\,\frac{d^2}{dz^2}\, G_{\ell+\frac{1}{2}}(z) \;-\; \frac{1}{z\sqrt{z}}\,\frac{d}{dz}\, G_{\ell+\frac{1}{2}}(z) \;+\; \frac{3}{4z^2\sqrt{z}}\, G_{\ell+\frac{1}{2}}(z) \tag{7.92}$$

one is lead to *Bessel's equation*

$$\left[\frac{d^2}{dz^2} \;+\; \frac{1}{z}\,\frac{d}{dz} \;-\; \frac{\nu^2}{z^2} \;+\; 1 \right] G_\nu(z) \;=\; 0 \tag{7.93}$$

where $\nu \;=\; \ell \,+\, \frac{1}{2}$. The regular solution of this equation is called the *regular Bessel function*. Its power expansion, using the conventional normalization, is given by [c.f. (7.79)]

$$J_\nu(z) \;=\; \left(\frac{z}{2}\right)^\nu \sum_{n=0}^{\infty} \frac{(iz/2)^{2n}}{n!\,\Gamma(\nu+n+1)}\;. \tag{7.94}$$

One can show that $J_{-\nu}(z)$, defined through (7.94), is also a solution of (7.93). This follows from the fact that ν appears in (7.93) only in the form ν^2. In the present case we consider solely the case $\nu \;=\; \ell \,+\, \frac{1}{2}$. In this case $J_{-\nu}(z)$ is linearly independent of $J_\nu(z)$ since the Wronskian

$$W(J_{\ell+\frac{1}{2}},\, J_{-\ell-\frac{1}{2}}) \;=\; (-1)^\ell\, \frac{2}{\pi z} \tag{7.95}$$

is non-vanishing. One can relate $J_{\ell+\frac{1}{2}}$ and $J_{-\ell-\frac{1}{2}}$ to the regular and irregular spherical Bessel functions. Comparision with (7.79) and (7.83) shows

$$j_\ell(z) \;=\; \sqrt{\frac{\pi}{2z}}\, J_{\ell+\frac{1}{2}}(z) \tag{7.96}$$

$$n_\ell(z) \;=\; (-1)^{\ell+1}\, \sqrt{\frac{\pi}{2z}}\, J_{-\ell-\frac{1}{2}}(z)\;. \tag{7.97}$$

These relationships are employed in case that since numerical algorithms provide the Bessel functions $J_\nu(z)$, but not directly the spherical Bessel functions $j_\ell(z)$ and $n_\ell(z)$.

Exercise 7.2.2: Demonstrate that expansion (7.94) is indeed a regular solution of (7.93). Adopt the procedures employed for the function $j_\ell(z)$.
Exercise 7.2.3: Prove the identity (7.95).

Generating Function of Spherical Bessel Functions

The stationary Schrödinger equation of free particles (7.43) has two solutions, namely, one given by (7.44, 7.45) and one given by (7.50). One can expand the former solution in terms of solutions (7.50). For example, in case of a free particle moving along the x_3-axis one expands

$$e^{ik_3x_3} \;=\; \sum_{\ell,m} a_{\ell m}\, j_\ell(kr)\, Y_{\ell m}(\theta,\phi)\ . \tag{7.98}$$

The l.h.s. can be written $\exp(ikr\cos\theta)$, i.e., the wave function does not depend on ϕ. In this case the expansion on the r.h.s. of (7.98) does not involve any non-vanishing m-values since $Y_{\ell m}(\theta,\phi)$ for non-vanishing m has a non-trivial ϕ-dependence as described by (5.106). Since the spherical harmonics $Y_{\ell 0}(\theta,\phi)$, according to (5.178) are given in terms of Legendre polynomials $P_\ell(\cos\theta)$ one can replace the expansion in (7.98) by

$$e^{ik_3x_3} \;=\; \sum_{\ell=0}^{\infty} b_\ell\, j_\ell(kr)\, P_\ell(\cos\theta)\ . \tag{7.99}$$

We want to determine the expansion coefficients b_ℓ.
The orthogonality properties (5.179) yield from (7.99)

$$\int_{-1}^{+1} d\cos\theta\; e^{ikr\cos\theta}\; P_\ell(\cos\theta) \;=\; b_\ell\, j_\ell(kr)\, \frac{2}{2\ell+1}\ . \tag{7.100}$$

Defining $x = \cos\theta$, $z = kr$, and using the Rodrigues formula for Legendre polynomials (5.150) one obtains

$$\int_{-1}^{+1} dx\; e^{izx}\; P_\ell(x) \;=\; \int_{-1}^{+1} dx\; e^{izx}\, \frac{1}{2^\ell \ell!}\, \frac{\partial^\ell}{\partial x^\ell}\,(x^2-1)^\ell\ . \tag{7.101}$$

Integration by parts yields

$$\begin{aligned}\int_{-1}^{+1} dx\; e^{izx}\; P_\ell(x) \;&=\; \frac{1}{2^\ell \ell!}\left[e^{izx}\, \frac{d^{\ell-1}}{dx^{\ell-1}}(x^2-1)^\ell \right]_{-1}^{+1} \\ &\quad -\, \frac{1}{2^\ell \ell!}\int_{-1}^{+1} dx\, \left(\frac{d}{dx}\, e^{izx}\right) \frac{d^{\ell-1}}{dx^{\ell-1}}\,(x^2-1)^\ell\ .\end{aligned} \tag{7.102}$$

One can show

$$\frac{d^{\ell-1}}{dx^{\ell-1}}(x^2-1)^\ell \;\sim\; (x^2-1)\,\times\,\text{polynomial in } x \tag{7.103}$$

and, hence, the surface term $\sim [\cdots]_{-1}^{+1}$ vanishes. This holds for ℓ consecutive integrations by part and one can conclude

$$\begin{aligned}\int_{-1}^{+1} dx\; e^{izx}\; P_\ell(x) \;&=\; \frac{(-1)^\ell}{2^\ell \ell!}\int_{-1}^{+1} dx\; (x^2-1)^\ell\, \frac{d^\ell}{dx^\ell}\, e^{izx} \\ &=\; \frac{(iz)^\ell}{2^\ell \ell!}\int_{-1}^{+1} dx\; (1-x^2)^\ell e^{izx}\ .\end{aligned} \tag{7.104}$$

Comparision with (7.100) gives

$$b_\ell \, j_\ell(kr) \, \frac{2}{2\ell \, + \, 1} \;=\; \frac{(iz)^\ell}{2^\ell \ell!} \int_{-1}^{+1} dx \, (1 \, - \, x^2)^\ell e^{izx} \; . \tag{7.105}$$

This expression allows one to determine the expansion coefficients b_ℓ. The identity (7.105) must hold for all powers of z, in particular, for the leading power x^ℓ [c.f. (7.69)]

$$b_\ell \, \frac{z^\ell}{1 \cdot 3 \cdot 5 \cdots (2\ell + 1)} \, \frac{2}{2\ell \, + \, 1} \;=\; \frac{(iz)^\ell}{2^\ell \ell!} \int_{-1}^{+1} dx \, (1 \, - \, x^2)^\ell \; . \tag{7.106}$$

Employing (5.117) one can write the r.h.s.

$$z^\ell \, i^\ell \, \frac{1}{2^\ell \ell!} \, \frac{(2\ell)!}{[1 \cdot 3 \cdot 5 \cdots (2\ell - 1)]^2} \, \frac{2}{2\ell + 1} \tag{7.107}$$

or

$$i^\ell \, (2\ell + 1) \, z^\ell \, \frac{1}{1 \cdot 3 \cdot 5 \cdots (2\ell + 1)} \, \frac{2}{2\ell + 1} \, \frac{(2\ell)!}{1 \cdot 2 \cdot 3 \cdot 4 \cdots (2\ell - 1) \cdot 2\ell} \tag{7.108}$$

where the last factor is equal to unity. Comparision with the l.h.s. of (7.106) yields finally

$$b_\ell \;=\; i^\ell \, (2\ell + 1) \tag{7.109}$$

or, after insertion into (7.99),

$$e^{ikr\cos\theta} \;=\; \sum_{\ell=0}^{\infty} i^\ell \, (2\ell + 1) \, j_\ell(kr) \, P_\ell(\cos\theta) \; . \tag{7.110}$$

One refers to the l.h.s. as the *generating function of the spherical Bessel functions.*

Integral Representation of Bessel Functions

Combining (7.105) and (7.109) results in the integral representation of $j_\ell(z)$

$$j_\ell(z) \;=\; \frac{(z)^\ell}{2^{\ell+1} \ell!} \int_{-1}^{+1} dx \, (1 \, - \, x^2)^\ell \, e^{izx} \; . \tag{7.111}$$

Employing (7.96) one can express this, using $\nu \;=\; \ell + \frac{1}{2}$,

$$J_\nu(z) \;=\; \frac{1}{\sqrt{\pi}\Gamma(\nu + \frac{1}{2})} \left(\frac{z}{2}\right)^\nu \int_{-1}^{+1} dx \, (1 \, - \, x^2)^{\nu - \frac{1}{2}} \, e^{izx} \; . \tag{7.112}$$

We want to consider the expression

$$G_\nu(z) \;=\; a_\nu z^\nu f_\nu(z) \tag{7.113}$$

where we define

$$f_\nu(z) \;=\; \int_C dt \, (1 \, - \, t^2)^{\nu - \frac{1}{2}} \, e^{izt} \; . \tag{7.114}$$

Here C is an integration path in the complex plane with endpoints t_1, t_2. $G_\nu(z)$, for properly chosen endpoints t_1, t_2 of the integration paths C, obeys Bessel's equation (7.93) for arbitrary ν. To prove this we note

$$f'_\nu(z) \;=\; i \int_C dt\,(1\,-\,t^2)^{\nu-\frac{1}{2}}\;t\,e^{izt}\,. \tag{7.115}$$

Integration by part yields

$$f'_\nu(z) \;=\; -\frac{i}{2\nu+1}\,\left[(1-t^2)^{\nu+\frac{1}{2}}\,e^{izt}\right]_{t_1}^{t_2} \;-\; \frac{z}{2\nu+1}\int_C dt\,(1\,-\,t^2)^{\nu+\frac{1}{2}}\,e^{izt}\,. \tag{7.116}$$

In case that the endpoints of the integration path C satisfy

$$\left[(1-t^2)^{\nu+\frac{1}{2}}\,e^{izt}\right]_{t_1}^{t_2} \;=\; 0 \tag{7.117}$$

one can write (7.116)

$$f'_\nu(z) \;=\; -\,\frac{z}{2\nu+1}\int_C dt\,(1\,-\,t^2)^{\nu-\frac{1}{2}}\,e^{izt} \;+\; \int_C dt\,(1\,-\,t^2)^{\nu-\frac{1}{2}}\;t^2\,e^{izt} \tag{7.118}$$

or

$$f'_\nu(z) \;=\; -\,\frac{z}{2\nu+1}\,\left[\,f_\nu(z)\;+\;f''_\nu(z)\right]\,. \tag{7.119}$$

From this we can conclude

$$f''_\nu(z) \;+\; \frac{2\nu+1}{z}\,f'_\nu(z) \;+\; f_\nu(z) \;=\; 0\,. \tag{7.120}$$

We note that equations (7.114, 7.120) imply also the property

$$(2\nu+1)\,f'_\nu(z) \;+\; z\,f_{\nu+1}(z) \;=\; 0\,. \tag{7.121}$$

Exercise 7.2.4: Prove (7.121).

We can now demonstrate that $G_\nu(z)$ defined in (7.113) obeys the Bessel equation (7.93) as long as the integration path in (7.113) satisfies (7.117). In fact, it holds for the derivatives of $G_\nu(z)$

$$G'_\nu(z) \;=\; \frac{\nu}{z}\,a_\nu z^\nu f_\nu(z) \;+\; a_\nu z^\nu f'_\nu(z) \tag{7.122}$$

$$G''(z) \;=\; \frac{\nu(\nu-1)}{z^2}\,a_\nu z^\nu f_\nu(z) \;+\; \frac{2\nu}{z}\,a_\nu z^\nu f'_\nu(z) \;+\; a_\nu z^\nu f''_\nu(z) \tag{7.123}$$

Insertion of these identities into Bessel's equation leads to a differential equation for $f_\nu(z)$ which is identical to (7.120) such that we can conclude that $G_\nu(z)$ for proper integration paths is a solution of (7.93).

We consider now the functions

$$u^{(j)}(z) \;=\; \frac{1}{\sqrt{\pi}\Gamma(\nu+\frac{1}{2})}\,\left(\frac{z}{2}\right)^\nu \int_{C_j} dx\,(1\,-\,x^2)^{\nu-\frac{1}{2}}\,e^{izx}\,,\quad j\;=\;1,2,3,4. \tag{7.124}$$

for the four integration paths in the complex plane parametrized as follows through a real path length s

$$C_1(t_1 = -1 \to t_2 = +1): \quad t = s \quad -1 \le s \le 1 \tag{7.125}$$

$$C_2(t_1 = 1 \to t_2 = 1 + i\,\infty): \quad t = 1 + is \quad 0 \le s < \infty \tag{7.126}$$

$$C_3(t_1 = 1 + i\,\infty \to t_2 = -1 + i\,\infty): \quad t = 1 + is \quad -1 \le s \le 1 \tag{7.127}$$

$$C_4(t_1 = -1 + i\,\infty \to t_1 = -1): \quad t = -1 + is \quad 0 \le s < \infty \tag{7.128}$$

$C = C_1 \cup C_2 \cup C_3 \cup C_4$ is a closed path. Since the integrand in (7.124) is analytical in the part of the complex plane surrounded by the path C we conclude

$$\sum_{j=1}^{4} u^{(j)}(z) \equiv 0 \tag{7.129}$$

The integrand in (7.124) vanishes along the whole path C_3 and, therefore, $u^{(3)}(z) \equiv 0$. Comparision with (7.112) shows $u^{(1)}(z) = J_\nu(z)$. Accordingly, one can state

$$J_\nu(z) = -\left[u^{(2)}(z) + u^{(4)}(z) \right] . \tag{7.130}$$

We note that the endpoints of the integration paths C_2 and C_4, for $\mathrm{Re} z > 0$ and $\nu \in \mathbb{R}$ obey (7.117) and, hence, $u^{(2)}(z)$ and $u^{(2)}(z)$ are both solutions of Bessel's equation (7.93).
Following convention, we introduce the so-called *Hankel functions*

$$H_\nu^{(1)}(z) = -2\, u^{(2)}(z) , \quad H_\nu^{(2)}(z) = -2\, u^{(4)}(z) . \tag{7.131}$$

According to (7.130) holds

$$J_\nu(z) = \frac{1}{2} \left[H_\nu^{(1)}(z) + H_\nu^{(2)}(z) \right] . \tag{7.132}$$

For $H_\nu^{(1)}(z)$ one derives, using $t = 1 + is$, $dt = i\,ds$, and

$$\begin{aligned} (1-t^2)^{\nu-\frac{1}{2}} e^{izt} &= [(1-t)(1+t)]^{\nu-\frac{1}{2}} e^{izt} \\ &= [-is(2+is)]^{\nu-\frac{1}{2}} e^{iz} e^{-zs} \\ &= e^{i(z-\pi\nu/2+\pi/4)} 2^{\nu-\frac{1}{2}} \, [s(1+is/2)]^{\nu-\frac{1}{2}} \, e^{-zs} , \end{aligned} \tag{7.133}$$

the integral expression

$$H_\nu^{(1)}(z) = e^{i(z-\pi\nu/2-\pi/4)} \, \frac{\sqrt{2}\, z^\nu}{\sqrt{\pi}\,\Gamma(\nu+\frac{1}{2})} \int_0^\infty ds\, [s(1+is/2)]^{\nu-\frac{1}{2}} \, e^{-zs} . \tag{7.134}$$

Similarly, one can derive

$$H_\nu^{(2)}(z) = e^{-i(z-\pi\nu/2-\pi/4)} \, \frac{\sqrt{2}\, z^\nu}{\sqrt{\pi}\,\Gamma(\nu+\frac{1}{2})} \int_0^\infty ds\, [s(1-is/2)]^{\nu-\frac{1}{2}} \, e^{-zs} . \tag{7.135}$$

(7.134) and (7.135) are known as the Poisson integrals of the Bessel functions.

Asymptotic Behaviour of Bessel Functions

We want to obtain now expansions of the Hankel functions $H^{(1,2)}_{\ell+\frac{1}{2}}(z)$ in terms of z^{-1} such that the expansions converge fast asymptotically, i.e., converge fast for $|z| \to \infty$. We employ for this purpose the Poisson integrals (7.134) and (7.135) which read for $\nu = \ell + \frac{1}{2}$

$$H^{(\frac{1}{2})}_{\ell+\frac{1}{2}}(z) \;=\; e^{\pm i[z-(\ell+1)\frac{\pi}{2}]} \sqrt{\frac{2z}{\pi}} \, \frac{z^\ell}{\ell!} \, f^{(\frac{1}{2})}_\ell(z) \tag{7.136}$$

where

$$f^{(\frac{1}{2})}_\ell(z) \;=\; \int_0^\infty ds \, [s(s \pm is/2)]^\ell \, e^{-zs} \,. \tag{7.137}$$

The binomial formula yields

$$f^{(\frac{1}{2})}_\ell(z) \;=\; \sum_{r=0}^{\ell} \binom{\ell}{r} \left(\pm\frac{i}{2}\right)^r \int_0^\infty ds \, s^{\ell+r} \, e^{-zs} \,. \tag{7.138}$$

The formula for the Laplace transform of s^n leads to

$$f^{(\frac{1}{2})}_\ell(z) \;=\; \sum_{r=0}^{\ell} \frac{(\ell+r)!\,\ell!}{r!(\ell-r)!} \left(\pm\frac{i}{2}\right)^r \left(\frac{1}{z}\right)^{\ell+r+1} \tag{7.139}$$

and, hence, we obtain

$$H^{(\frac{1}{2})}_{\ell+\frac{1}{2}}(z) \;=\; \sqrt{\frac{2}{\pi z}} \, e^{\pm i[z-(\ell+1)\frac{\pi}{2}]} \sum_{r=0}^{\ell} \frac{(\ell+r)!}{r!(\ell-r)!} \left(\pm\frac{i}{2z}\right)^r \tag{7.140}$$

Bessel Functions with Negative Index

Since ν enters the Bessel equation (7.93) only as ν^2, $H^{(1)}_\nu(z)$ as well as $H^{(1)}_{-\nu}(z)$ are solutions of this equation. As a second order differential equation the Bessel equation has two linearly independent solutions. For such solutions $g(z)$, $h(z)$ to be linearly independent, the Wronskian $W(g,h)$ must be a non-vanishing function.
For the Wronskian connected with the Bessel equation (7.93) holds the identity

$$W' \;=\; -\frac{1}{z}\,W \tag{7.141}$$

the derivation of which follows the derivation on page 192 for the Wronskian of the radial Schrödinger equation. The general solution of (7.141) is

$$W(z) \;=\; -\frac{c}{z} \,. \tag{7.142}$$

In case of $g(z) = H^{(1)}_{\ell+\frac{1}{2}}(z)$ and $h(z) = H^{(2)}_{\ell+\frac{1}{2}}(z)$ one can identify the constant c by using the leading terms in the expansions (7.140). One obtains

$$W(z) \;=\; -\frac{4i}{\pi z} \,, \tag{7.143}$$

i.e., $H^{(1,2)}_{\ell+\frac{1}{2}}(z)$ are, in fact, linearly independent.
One can then expand

$$H^{(1)}_{-\nu}(z) \;=\; A\,H^{(1)}_{\ell+\frac{1}{2}}(z) \;+\; B\,H^{(2)}_{\ell+\frac{1}{2}}(z)\;. \tag{7.144}$$

The expansion coefficients A, B can be obtained from the asymptotic expansion (7.140). For $|z| \to \infty$ the leading terms yield

$$\frac{1}{\sqrt{z}}\,e^{i(z+\frac{\ell\pi}{2})} \;=\; \frac{1}{\sqrt{z}}\,A\,e^{i(z-\frac{\ell\pi}{2}-\frac{\pi}{2})} \;+\; \frac{1}{\sqrt{z}}\,B\,e^{-i(z-\frac{\ell\pi}{2}-\frac{\pi}{2})} \quad |z| \;\to\; \infty\;. \tag{7.145}$$

This equation can hold only for $B \,=\, 0$ and $A \,=\, \exp[i(\ell + \frac{1}{2})\pi]$. We conclude

$$H^{(1)}_{-(\ell+\frac{1}{2})}(z) \;=\; i\,(-1)^{\ell}\,H^{(1)}_{\ell+\frac{1}{2}}(z)\;. \tag{7.146}$$

Simarly, one can show

$$H^{(2)}_{-(\ell+\frac{1}{2})}(z) \;=\; -i\,(-1)^{\ell}\,H^{(2)}_{\ell+\frac{1}{2}}(z)\;. \tag{7.147}$$

Spherical Hankel Functions

In analogy to equations (7.90, 7.97) one defines the spherical Hankel functions

$$h^{(1,2)}_{\ell}(z) \;=\; \sqrt{\frac{\pi}{2z}}\;H^{(1,2)}_{\ell+\frac{1}{2}}(z)\;. \tag{7.148}$$

Following the arguments provided above (see page 193) the functions $h^{(1,2)}_{\ell}(z)$ are solutions of the radial Schrödinger equation of free particles (7.53). According to (7.96, 7.132, 7.148) holds for the regular spherical Bessel function

$$j_{\ell}(z) \;=\; \frac{1}{2}\,[\,h^{(1)}_{\ell}(z) \;+\; h^{(2)}_{\ell}(z)\,]\;. \tag{7.149}$$

We want to establish also the relationship between $h^{(1,2)}_{\ell}(z)$ and the irregular spherical Bessel function $n_{\ell}(z)$ defined in (7.97). From (7.97, 7.132) follows

$$n_{\ell}(z) \;=\; \frac{1}{2}\sqrt{\frac{\pi}{2z}}\,(-1)^{\ell+1}\,\left[H^{(1)}_{-(\ell+\frac{1}{2})}(z) \;+\; H^{(2)}_{-(\ell+\frac{1}{2})}(z)\right]\;. \tag{7.150}$$

According to (7.146, 7.147) this can be written

$$n_{\ell}(z) \;=\; \frac{1}{2i}\,\left[h^{(1)}_{\ell}(z) \;-\; h^{(2)}_{\ell}(z)\right]\;. \tag{7.151}$$

Equations (7.149, 7.151) are equivalent to

$$h^{(1)}_{\ell}(z) \;=\; j_{\ell}(z) \;+\; i\,n_{\ell}(z) \tag{7.152}$$

$$h^{(2)}_{\ell}(z) \;=\; j_{\ell}(z) \;-\; i\,n_{\ell}(z)\;. \tag{7.153}$$

Asymptotic Behaviour of Spherical Bessel Functions

We want to derive now the asymptotic behaviour of the spherical Bessel functions $h_\ell^{(1,2)}(z)$, $j_\ell(z)$ and $n_\ell(z)$. From (7.140) and (7.148) one obtains readily

$$h_\ell^{(\frac{1}{2})}(z) \;=\; \frac{(\mp i)^{\ell+1}}{z}\, e^{\pm iz} \sum_{r=0}^{\ell} \frac{(\ell+r)!}{r!(\ell-r)!} \left(\pm\frac{i}{2z}\right)^r \tag{7.154}$$

The leading term in this expansion, at large $|z|$, is

$$h_\ell^{(\frac{1}{2})}(z) \;=\; \frac{(\mp i)^{\ell+1}}{z}\, e^{\pm iz}\,. \tag{7.155}$$

To determine $j_\ell(z)$ and $n_\ell(z)$ we note that for $z \in \mathbb{R}$ the spherical Hankel functions $h_\ell^{(1)}(z)$ and $h_\ell^{(2)}(z)$, as given by (7.140, 7.148), are complex conjugates. Hence, it follows

$$z \in \mathbb{R} \;:\quad j_\ell(z) \;=\; \mathrm{Re}[h_\ell^{(1)}(z)]\,, \quad n_e ll(z) \;=\; \mathrm{Im}[h_\ell^{(1)}(z)]\,. \tag{7.156}$$

Using

$$p_\ell(z) \;=\; \mathrm{Re}\sum_{r=0}^{\ell} \frac{(\ell+r)!}{r!(\ell-r)!}\left(\frac{i}{2z}\right)^r \;=\; \sum_{r=0}^{[\ell/2]} \frac{(\ell+2r)!}{(2r)!(\ell-2r)!}\left(\frac{-1}{4z^2}\right)^r \tag{7.157}$$

$$\begin{aligned} \frac{i}{2z}\, q_\ell(z) \;&=\; i\,\mathrm{Im}\sum_{r=0}^{\ell} \frac{(\ell+r)!}{r!(\ell-r)!}\left(\frac{i}{2z}\right)^r \\ &=\; \begin{cases} \frac{i}{2z} \sum_{r=0}^{[\ell-1/2]} \frac{(\ell+2r+1)!}{(2r+1)!(\ell-2r-1)!}\left(\frac{-1}{4z^2}\right)^r & \ell \,\geq\, 1 \\ 0 & \ell \,=\, 0 \end{cases} \end{aligned} \tag{7.158}$$

one can derive then from (7.154) the identities

$$j_\ell(z) \;=\; \frac{\cos[z \,-\, (\ell+1)\frac{\pi}{2}]}{z}\, p_\ell(z) \;-\; \frac{\sin[z \,-\, (\ell+1)\frac{\pi}{2}]}{2z^2}\, q_\ell(z) \tag{7.159}$$

$$n_\ell(z) \;=\; \frac{\cos[z \,-\, (\ell+1)\frac{\pi}{2}]}{2z^2}\, q_\ell(z) \;+\; \frac{\cos(z-\ell\pi/2)}{z}\, p_\ell(z)\,. \tag{7.160}$$

Employing $\cos[z \,-\, (\ell+1)\frac{\pi}{2}]\,. = \sin(z-\ell\pi/2)$ and $\sin[z \,-\, (\ell+1)\frac{\pi}{2}]\,. = -\cos(z-\ell\pi/2)$ results in the alternative expressions

$$j_\ell(z) \;=\; \frac{\sin(z-\ell\pi/2)}{z}\, p_\ell(z) \;+\; \frac{\cos(z-\ell\pi/2)}{2z^2}\, q_\ell(z) \tag{7.161}$$

$$n_\ell(z) \;=\; \frac{\sin(z-\ell\pi/2)}{2z^2}\, q_\ell(z) \;-\; \frac{\cos(z-\ell\pi/2)}{z}\, p_\ell(z)\,. \tag{7.162}$$

The leading terms in these expansions, at large $|z|$, are

$$j_\ell(z) \;=\; \frac{\sin(z-\ell\pi/2)}{z} \tag{7.163}$$

$$n_\ell(z) \;=\; -\,\frac{\cos(z-\ell\pi/2)}{z}\,. \tag{7.164}$$

Expressions for the Spherical bessel Functions $j_\ell(z)$ and $n_\ell(z)$

The identities (7.161, 7.162) allow one to provide explicit expressions for $j_\ell(z)$ and $n_\ell(z)$. One obtains for $\ell = 0, 1, 2$

$$j_0(z) = \frac{\sin z}{z} \tag{7.165}$$

$$n_0(z) = -\frac{\cos z}{z} \tag{7.166}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z} \tag{7.167}$$

$$n_1(z) = -\frac{\cos z}{z^2} - \frac{\sin z}{z} \tag{7.168}$$

$$j_2(z) = \left(\frac{3}{z^3} - \frac{1}{z}\right)\sin z - \frac{3}{z^2}\cos z \tag{7.169}$$

$$n_2(z) = \left(-\frac{3}{z^3} + \frac{1}{z}\right)\cos z - \frac{3}{z^2}\sin z \tag{7.170}$$

Recursion Formulas of Spherical Bessel Functions

The spherical Bessel functions obey the recursion relationships

$$g_{\ell+1}(z) = \frac{\ell}{z}\, g_\ell(z) - g'_\ell(z) \tag{7.171}$$

$$g_{\ell+1}(z) = \frac{2\ell+1}{z}\, g_\ell(z) - g_{\ell-1}(z) \tag{7.172}$$

where $g_\ell(z)$ is either of the functions $h_\ell^{(1,2)}(z)$, $j_\ell(z)$ and $n_\ell(z)$. One can combine (7.171, 7.172) to obtain the recursion relationship

$$\begin{pmatrix} g_{\ell+1}(z) \\ g'_{\ell+1}(z) \end{pmatrix} = \mathbf{A}_\ell(z) \begin{pmatrix} g_\ell(z) \\ g'_\ell(z) \end{pmatrix} \tag{7.173}$$

$$\mathbf{A}_\ell(z) = \begin{pmatrix} \frac{\ell}{z} & -1 \\ 1 - \frac{\ell(\ell+1)}{z^2} & \frac{\ell+2}{z} \end{pmatrix} \tag{7.174}$$

We want to prove these relationships. For this purpose we need to demonstrate only that the relationships hold for $g_\ell(z) = h_\ell^{(1,2)}(z)$. From the linearity of the relationships (7.171–7.174) and from (7.149, 7.151) follows then that the relatiosnhips hold also for $g_\ell(z) = j_\ell(z)$ and $g_\ell(z) = n_\ell(z)$. To demonstrate that (7.171) holds for $g_\ell(z) = h_\ell^{(1,2)}(z)$ we employ (7.124, 7.131, 7.148) and express

$$g_\ell(z) = h_\ell^{(1,2)}(z) = -2\sqrt{\frac{\pi}{2z}}\ \frac{1}{\sqrt{\pi}\,\Gamma(\nu+\frac{1}{2})}\left(\frac{z}{2}\right)^\nu \int_{C_{2,4}} dx\,(1 - x^2)^{\nu-\frac{1}{2}}\, e^{izx}\,. \tag{7.175}$$

Using $\Gamma(\ell+1) = \ell!$, defining $a = -1$ and employing $f_\nu(z)$ as defined in (7.114) we can write

$$g_\ell(z) = a\,\frac{z^\ell}{2^\ell \ell!}\, f_{\ell+\frac{1}{2}}(z)\,. \tag{7.176}$$

The derivative of this expression is

$$g'_\ell(z) \;=\; \frac{\ell}{z}\, g_\ell(z) \;+\; a\, \frac{z^\ell}{2^\ell \ell!}\, f'_{\ell+\frac{1}{2}}(z) \;. \tag{7.177}$$

Employing (7.121), i.e.,

$$f'_{\ell+\frac{1}{2}}(z) \;=\; -\,\frac{z}{2\ell+2}\, f_{\ell+\frac{3}{2}}(z) \;, \tag{7.178}$$

yields, together with (7.176)

$$g'_\ell(z) \;=\; \frac{\ell}{z}\, g_\ell(z) \;-\; g_{\ell+1}(z) \tag{7.179}$$

from which follows (7.171).
In order to prove (7.172) we differentiate (7.179)

$$g''_\ell(z) \;=\; -\,\frac{\ell}{z^2}\, g_\ell(z) \;+\; \frac{\ell}{z}\, g'_\ell(z) \;-\; g'_{\ell+1}(z) \;. \tag{7.180}$$

Since $g_\ell(z)$ is a solution of the radial Schrödinger equation (7.58) it holds

$$g''_\ell(z) \;=\; -\frac{2}{z}\, g'_\ell(z) \;+\; \frac{\ell(\ell+1)}{z^2}\, g_\ell(z) \;-\; g_\ell(z) \;. \tag{7.181}$$

Using this identity to replace the second derivative in (7.180) yields

$$g'_{\ell+1}(z) \;=\; g_\ell(z) \;-\; \frac{\ell(\ell+2)}{z^2}\, g_\ell(z) \;+\; \frac{\ell+2}{z}\, g'_\ell(z) \;. \tag{7.182}$$

Replacing all first derivatives employing (7.179) leads to (7.172).
To prove (7.173, 7.174) we start from (7.171). The first component of (7.173), in fact, is equivalent to (7.171). The second component of (7.173) is equivalent to (7.182).

Exercise 7.2.5: Provide a detailed derivation of (7.172).
Exercise 7.2.6: Employ the recursion relationship (7.173, 7.174) to determine (a) $j_1(z)$, $j_2(z)$ from $j_0(z)$, $j'_0(z)$ using (7.165), and (b) $n_1(z)$, $n_2(z)$ from $n_0(z)$, $n'_0(z)$ using (7.166).
