Chapter 2
Elastic Scattering by a Conservative Potential

2.1 Scattering Amplitude and Scattering Cross Section

In quantum mechanics the relative motion of a projectile and a target is described by a complex-valued wave function ψ which depends on the relative distance $\mathbf{r}$ of the projectile from the target. The wave function is assumed to obey the time-independent Schrödinger equation for a particle with (reduced) mass μ in the potential $V(\mathbf{r})$,

$$\left[-\frac{\hbar^2}{2\mu}\Delta + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}). \tag{2.1}$$

In order to describe elastic scattering at energy $E = \hbar^2 k^2/(2\mu)$, we look for solutions of (2.1), which at large distances obey boundary conditions corresponding to an incoming plane wave and an outgoing, scattered spherical wave, as sketched in Fig. 2.1,

$$\psi(\mathbf{r}) \overset{r\to\infty}{\sim} \mathrm{e}^{\mathrm{i}kz} + f(\theta,\phi)\frac{\mathrm{e}^{\mathrm{i}kr}}{r}. \tag{2.2}$$

Although a real scattering event is a time-dependent process, the description via stationary solutions of the time-independent Schrödinger equation is adequate in most experimental situations [30]. The explicit form of the two terms on the right-hand side of (2.2) implies that the motion of the particle is asymptotically ($r \to \infty$) free, which places some constraints on the large-distance behaviour of the potential $V(\mathbf{r})$. Unless stated otherwise, we assume that the potential falls off faster than $1/r^2$ at large distances, $r^2 V(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} 0$.

The particle flux associated with the quantum mechanical wave function is described via the *current density* $\mathbf{j}(\mathbf{r})$. Classically, $\mathbf{j}(\mathbf{r})$ would be the product of particle density and velocity. In the corresponding quantum mechanical expression, the velocity is replaced by $\hat{\mathbf{p}}/\mu$, where $\hat{\mathbf{p}} = (\hbar/\mathrm{i})\nabla$ is the momentum operator conjugate

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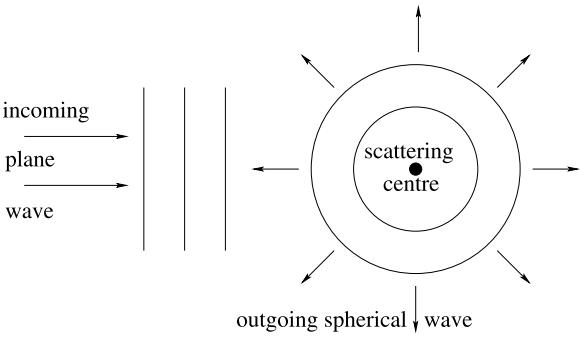

Fig. 2.1 Schematic illustration of the incoming plane wave and the outgoing spherical wave as described by a solution of (2.1) obeying the boundary conditions (2.2)

to $\mathbf{r}$,

$$\mathbf{j}(\mathbf{r}) = \Re\left[\psi^*(\mathbf{r})\frac{\hat{\mathbf{p}}}{\mu}\psi(\mathbf{r})\right] = \frac{\hbar}{2\mathrm{i}\mu}\psi^*(\mathbf{r})\nabla\psi(\mathbf{r}) + \mathrm{cc}; \tag{2.3}$$

"cc" stands for the complex conjugate of the preceding term.

From the first term on the right-hand side of (2.2) we find that the current density associated with the incoming plane wave is $\mathbf{j}_{\mathrm{in}} = \hat{\mathbf{e}}_z \hbar k/\mu$, corresponding to a wave of unit spatial density moving with velocity $v = \hbar k/\mu$ in the direction of $\hat{\mathbf{e}}_z$, the unit vector in z-direction. The second term on the right-hand side of (2.2) describes an outgoing spherical wave, modulated by the *scattering amplitude* $f(\theta, \phi)$, which has the physical dimensions of a length. Inserted in (2.3) this term generates an outgoing current density which is given to leading order by

$$\mathbf{j}_{\mathrm{out}}(\mathbf{r}) = \frac{\hbar k}{\mu}\left|f(\theta,\phi)\right|^2 \frac{\hat{\mathbf{e}}_{\mathbf{r}}}{r^2} + O\left(\frac{1}{r^3}\right), \tag{2.4}$$

where $\hat{\mathbf{e}}_{\mathbf{r}} = \mathbf{r}/r$ is the radial unit vector. Asymptotically, the flux of particle density scattered into the solid angle $\mathrm{d}\Omega = \sin\theta \mathrm{d}\theta\mathrm{d}\phi$ is $\lim_{r\to\infty}\mathbf{j}_{\mathrm{out}}(\mathbf{r})\cdot\mathrm{d}\mathbf{s}$ with $\mathrm{d}\mathbf{s} = \hat{\mathbf{e}}_{\mathbf{r}} r^2 \mathrm{d}\Omega$, i.e., $(\hbar k/\mu)|f(\theta,\phi)|^2\mathrm{d}\Omega$. The differential scattering cross section is given by this flux, normalized to the incoming current density $|\mathbf{j}_{\mathrm{in}}| = \hbar k/\mu$,

$$\mathrm{d}\sigma = \left|f(\theta,\phi)\right|^2 \mathrm{d}\Omega, \qquad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left|f(\theta,\phi)\right|^2. \tag{2.5}$$

Integrating over all directions θ, ϕ yields the *integrated* or *total* elastic scattering cross section,

$$\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega = \int_0^{2\pi}\mathrm{d}\phi \int_0^{\pi} \sin\theta \mathrm{d}\theta \left|f(\theta,\phi)\right|^2. \tag{2.6}$$

As in the classical case, see Eqs. (1.37), (1.38) in Sect. 1.3, σ has the physical dimensions of an area; $\mathrm{d}\sigma$ can be interpreted as the area in the plane perpendicular to the direction of incidence, through which the incoming flux passes which is scattered into the outgoing direction $\mathrm{d}\Omega$. Correspondingly, σ describes the area through which all the flux passes which is scattered at all.

Each solution of the stationary Schrödinger equation (2.1) fulfills the *continuity equation* in the form,

$$\nabla \cdot \mathbf{j} = -\frac{\partial \rho}{\partial t} = 0, \quad \text{or, equivalently,} \quad \oint \mathbf{j} \cdot \mathrm{d}\mathbf{s} = 0. \tag{2.7}$$

This states that the net flux through any closed surface vanishes, which is an expression of particle conservation. For the surface of a large sphere with radius $r \to \infty$, the integrated contribution from the incoming plane wave, $I_{\text{in}} = \oint \mathbf{j}_{\text{in}} \cdot \mathrm{d}\mathbf{s}$, vanishes because of symmetry. The contribution I_{out} from the outgoing current density is positive unless the scattering amplitude $f(\theta, \phi)$ vanishes identically,

$$I_{\text{out}} = \lim_{r\to\infty} \oint \mathbf{j}_{\text{out}}(\mathbf{r}) \cdot \mathrm{d}\mathbf{s} = \frac{\hbar k}{\mu} \int \left| f(\Omega) \right|^2 \mathrm{d}\Omega = \frac{\hbar k}{\mu}\sigma. \tag{2.8}$$

The fact that $I_{\text{in}} + I_{\text{out}}$ does not vanish does not contradict Eq. (2.7), because the total current density $\mathbf{j}$ is not merely the sum of $\mathbf{j}_{\text{in}}$ and $\mathbf{j}_{\text{out}}$, but contains a contribution from the interference of plane and spherical waves,

$$\mathbf{j}(\mathbf{r}) \overset{r\to\infty}{\sim} \mathbf{j}_{\text{in}} + \mathbf{j}_{\text{out}}(r) + \mathbf{j}_{\text{int}}(r). \tag{2.9}$$

The interference term is, including terms up to $O(1/r^2)$,

$$\mathbf{j}_{\text{int}}(r) \overset{r\to\infty}{\sim} \frac{\hbar}{2\mu} f(\theta,\phi) \left[k \frac{\mathrm{e}^{\mathrm{i}k(r-z)}}{r} (\hat{\mathbf{e}}_{\mathbf{r}} + \hat{\mathbf{e}}_z) + \mathrm{i} \frac{\mathrm{e}^{\mathrm{i}k(r-z)}}{r^2} \hat{\mathbf{e}}_{\mathbf{r}} \right] + \text{cc} + \cdots, \tag{2.10}$$

where $\cdots$ stands for vector contributions orthogonal to $\hat{\mathbf{e}}_{\mathbf{r}}$. The contribution of this interference term to the flux through the surface element $\mathrm{d}\mathbf{s} = \hat{\mathbf{e}}_{\mathbf{r}} r^2 \mathrm{d}\Omega$ of a sphere with large radius r is,

$$\mathbf{j}_{\text{int}}(r) \cdot \mathrm{d}\mathbf{s} = \frac{\hbar}{2\mu} f(\theta,\phi) \mathrm{e}^{\mathrm{i}kr(1-\cos\theta)} \big[kr(1+\cos\theta) + \mathrm{i} \big] \mathrm{d}\Omega + \text{cc}. \tag{2.11}$$

The contribution $I_{\text{int}} = \lim_{r\to\infty} \oint \mathbf{j}_{\text{int}}(\mathbf{r}) \cdot \mathrm{d}\mathbf{s}$ to the total flux through the surface of the sphere with large radius r is obtained by integrating the expression (2.11) over $\mathrm{d}\Omega$ and taking the limit $r \to \infty$. The contribution due to the "i" in the square bracket vanishes, because $\lim_{\gamma\to\infty} \int_{-1}^{1} f(x) \mathrm{e}^{\mathrm{i}\gamma(1-x)} \mathrm{d}x = 0$, with $kr \equiv \gamma$, $x = \cos\theta$. A non-vanishing result is obtained from the preceding term proportional to kr via the identity

$$\lim_{\gamma\to\infty} \gamma \int_{-1}^{+1} (1+x) f(x) \mathrm{e}^{\mathrm{i}\gamma(1-x)} \mathrm{d}x = 2\mathrm{i} f(1), \quad \text{namely,} \tag{2.12}$$

$$\begin{aligned} I_{\text{int}} &= \lim_{r\to\infty} \int_0^{2\pi} \mathrm{d}\phi \int_{-1}^{+1} \mathrm{d}\cos\theta \, \mathbf{j}_{\text{int}}(r) \cdot \mathrm{d}\mathbf{s} \\ &= \frac{\hbar}{\mu} 2\pi \mathrm{i} f(\theta = 0) + \text{cc} = -\frac{\hbar}{\mu} 4\pi \Im\big[f(\theta = 0) \big]. \end{aligned} \tag{2.13}$$

Particle conservation requires that I_{int} exactly cancels the contribution I_{out} as given in (2.8), so

$$\sigma = \frac{4\pi}{k}\Im\big[f(\theta = 0)\big]. \tag{2.14}$$

Equation (2.14) is known as the *optical theorem*. It shows that destructive interference between the plane wave and the scattered wave in the forward direction $\theta = 0$ compensates the loss of flux through the scattering process. Note that $f(\theta, \phi)$ becomes independent of ϕ for $\theta = 0$.

2.2 Lippmann–Schwinger Equation and Born Approximation

The Schrödinger equation (2.1) can be rewritten as

$$\left(E + \frac{\hbar^2}{2\mu}\Delta\right)\psi(\mathbf{r}) = V(\mathbf{r})\psi(\mathbf{r}) \tag{2.15}$$

and transformed into an integral equation with the help of the *free-particle Green's function* $\mathcal{G}(\mathbf{r}, \mathbf{r}')$, which fulfills

$$\left(E + \frac{\hbar^2}{2\mu}\Delta_{\mathbf{r}}\right)\mathcal{G}\big(\mathbf{r}, \mathbf{r}'\big) = \delta\big(\mathbf{r} - \mathbf{r}'\big) \tag{2.16}$$

and is explicitly given by

$$\mathcal{G}(\mathbf{r}, \mathbf{r}') = -\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}k|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}. \tag{2.17}$$

A wave function $\psi(\mathbf{r})$ obeying the integral equation

$$\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}kz} + \int \mathcal{G}(\mathbf{r}, \mathbf{r}')V(\mathbf{r}')\psi(\mathbf{r}')\mathrm{d}\mathbf{r}' \tag{2.18}$$

necessarily obeys the Schrödinger equation (2.15). This would also hold, if the first term $\mathrm{e}^{\mathrm{i}kz}$ were replaced by $\mathrm{e}^{-\mathrm{i}kz}$ or any other solution of the "homogeneous" version, $[E + (\hbar^2/(2\mu))\Delta]\psi(\mathbf{r}) = 0$, of Eq. (2.15).[1]

Equation (2.18) is called the *Lippmann–Schwinger equation*. It is essentially equivalent to the Schrödinger equation (2.1), but has the advantage, that the boundary conditions (2.2) are automatically fulfilled. To see this we make use of the explicit form of the Green's function (2.17) for $|\mathbf{r}| \gg |\mathbf{r}'|$:

$$\mathcal{G}\big(\mathbf{r}, \mathbf{r}'\big) = -\frac{\mu}{2\pi\hbar^2}\frac{\mathrm{e}^{\mathrm{i}kr}}{r}\left[\mathrm{e}^{-\mathrm{i}\mathbf{k}_{\mathbf{r}}\cdot\mathbf{r}'} + O\left(\frac{r'}{r}\right)\right], \tag{2.19}$$

[1] Equation (2.15) is homogeneous, whether or not the right-hand side is replaced by zero. The present terminology is adapted from applications to genuinely inhomogeneous differential equations, where the right-hand side is a given function independent of the solution being sought.

where $\mathbf{k_r} = k\hat{\mathbf{e}}_\mathbf{r}$ is the wave vector which has the same length as the wave vector $k\hat{\mathbf{e}}_z$ of the incoming plane wave but points in the direction of the radial vector $\hat{\mathbf{e}}_\mathbf{r}$ (without prime). Inserting (2.19) into (2.18) gives the asymptotic form (2.2) with

$$f(\theta,\phi) = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{e}^{-\mathrm{i}\mathbf{k_r}\cdot\mathbf{r}'}\,V(\mathbf{r}')\psi(\mathbf{r}')\mathrm{d}\mathbf{r}'. \tag{2.20}$$

Equation (2.20) is an exact expression for the scattering amplitude f, but its evaluation requires the knowledge of the exact solution ψ of the Schrödinger (or Lippmann–Schwinger) equation. If, in addition to fulfilling $r^2V(\mathbf{r}) \overset{r\to\infty}{\longrightarrow} 0$, the potential is less singular than $1/r^2$ at the origin, $r^2V(\mathbf{r}) \overset{r\to 0}{\longrightarrow} 0$ (and a continuous function of $\mathbf{r}$), then the integral on the right-hand side of (2.20) converges for all values of $\mathbf{k_r}$.

If the influence of the potential V can be regarded to be small, the Lippmann–Schwinger equation (2.20) can be used to construct a perturbation series. Inserting the explicit form (2.18) for $\psi(\mathbf{r}')$ into (2.20) gives

$$\begin{aligned} f(\theta,\phi) = -\frac{\mu}{2\pi\hbar^2}\Bigg[&\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{k_r}\cdot\mathbf{r}'}V(\mathbf{r}')\mathrm{e}^{\mathrm{i}kz'} \\ &+ \int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{k_r}\cdot\mathbf{r}'}V(\mathbf{r}')\int \mathrm{d}\mathbf{r}''\mathscr{G}(\mathbf{r}',\mathbf{r}'')V(\mathbf{r}'')\psi(\mathbf{r}'')\Bigg]. \end{aligned} \tag{2.21}$$

Repeatedly inserting the explicit form (2.18) for the exact wave function ψ generates a series of approximations ordered by the number of times the potential V appears in the (multiple) integral. This series is called the *Born series*. Keeping only the first term on the upper line of Eq. (2.21) defines the *Born approximation* in first order,

$$f^{\mathrm{Born}}(\theta,\phi) = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{k_r}\cdot\mathbf{r}'}V(\mathbf{r}')\mathrm{e}^{\mathrm{i}kz'} = -\frac{\mu}{2\pi\hbar^2}\int \mathrm{d}\mathbf{r}'\mathrm{e}^{-\mathrm{i}\mathbf{q}\cdot\mathbf{r}'}V(\mathbf{r}'), \tag{2.22}$$

where $\hbar\mathbf{q}$ is the momentum transferred from the incoming wave travelling in the direction of $\hat{\mathbf{e}}_z$ to the outgoing wave travelling in the direction of $\hat{\mathbf{e}}_\mathbf{r}$,

$$\mathbf{q} = k(\hat{\mathbf{e}}_\mathbf{r} - \hat{\mathbf{e}}_z). \tag{2.23}$$

The scattering amplitude in Born approximation is essentially the Fourier transform of the potential; its dependence on the scattering angle(s) enters through the wave vector of momentum transfer (2.23). The polar angle θ is related to the wave number $q = |\mathbf{q}|$ via

$$q = 2k\sin(\theta/2), \tag{2.24}$$

see Fig. 2.2. If the potential V is real and radially symmetric, $V = V(r)$, then f^{Born} is a real function depending only on the wave number q. The scattering amplitude in Born approximation thus necessarily violates the optical theorem (2.14).

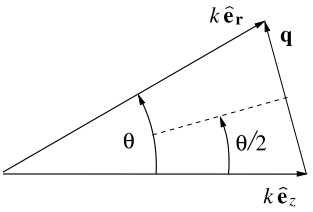

Fig. 2.2 Illustration of the relation (2.24) connecting the polar angle θ with the wave vector $\mathbf{q}$ of momentum transfer

Inserting $e^{ikz''}$ for $\psi(\mathbf{r}'')$ in the integral in the lower line of Eq. (2.21) defines the *second-order Born approximation*. Including the contribution $\int \mathscr{G}(\mathbf{r}'', \mathbf{r}''')V(\mathbf{r}''')d\mathbf{r}'''$ paves the way to higher-order terms.

2.3 Radially Symmetric Potentials

2.3.1 Angular Momentum

When the potential is radially symmetric, $V(\mathbf{r}) = V(r)$, the orbital angular momentum $\hat{\mathbf{L}} = \mathbf{r} \times \hat{\mathbf{p}}$ is a conserved quantity. The three components of $\hat{\mathbf{L}}$ commute with $\hat{\mathbf{L}}^2$ but not with each other, $[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$. The space of angular functions can be spanned by simultaneous eigenstates of $\hat{\mathbf{L}}^2$ and one component of $\hat{\mathbf{L}}$, which is usually chosen to be $\hat{L}_z$. In coordinate representation, these states are the *spherical harmonics* $Y_{l,m}(\theta, \phi)$, which are labelled by the angular momentum quantum number l and the azimuthal quantum number m,

$$\begin{aligned} &\hat{\mathbf{L}}^2 Y_{l,m}(\theta,\phi) = l(l+1)\hbar^2 Y_{l,m}(\theta,\phi), \quad l = 0, 1, 2, \ldots; \\ &\hat{L}_z Y_{l,m}(\theta,\phi) = m\hbar Y_{l,m}(\theta,\phi), \quad m = -l, -l+1, \ldots, l-1, l. \end{aligned} \tag{2.25}$$

The general structure[2] of the spherical harmonics is,

$$Y_{l,m}(\theta,\phi) = e^{im\phi} \sin^{|m|}(\theta) \mathrm{Pol}_{l-|m|}(\cos\theta), \tag{2.26}$$

where $\mathrm{Pol}_\lambda(x)$ stands for a polynomial of degree λ in x. They are orthonormal,

$$\begin{aligned} \int Y_{l,m}(\Omega)^* Y_{l',m'}(\Omega) d\Omega &= \int_0^{2\pi} d\phi \int_{-1}^{+1} d\cos\theta \, Y_{l,m}(\theta,\phi)^* Y_{l',m'}(\theta,\phi) \\ &= \delta_{l,l'}\delta_{m,m'}, \end{aligned} \tag{2.27}$$

and obey the following relations:

$$Y_{l,m}(\theta - \pi, \phi + \pi) = Y_{l,-m}(\theta,\phi) = (-1)^l Y_{l,m}(\theta,\phi). \tag{2.28}$$

[2] For precise definitions of the $Y_{l,m}$ and other special functions see Appendix B.

For vanishing azimuthal quantum number, $m = 0$, the spherical harmonics do not depend on ϕ and are proportional to *Legendre polynomials* [1] of $\cos\theta$,

$$Y_{l,m=0}(\theta) = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\theta). \tag{2.29}$$

The Legendre polynomials fulfill the orthogonality relation

$$\int_{-1}^{1} P_l(x) P_{l'}(x) \mathrm{d}x = \frac{2}{2l+1} \delta_{l,l'}, \tag{2.30}$$

and for two vectors $\mathbf{a}$, $\mathbf{b}$, with $|\mathbf{a}| \leq |\mathbf{b}|$ we have

$$\frac{1}{|\mathbf{a}-\mathbf{b}|} = \sum_{l=0}^{\infty} \frac{|\mathbf{a}|^l}{|\mathbf{b}|^{l+1}} P_l(\cos\theta), \tag{2.31}$$

where θ is the angle between $\mathbf{a}$ and $\mathbf{b}$. For $|\mathbf{a}| = |\mathbf{b}|$ Eq. (2.31) yields

$$\sum_{l=0}^{\infty} P_l(\cos\theta) = \frac{1}{2\sin(\theta/2)}. \tag{2.32}$$

2.3.2 Partial-Waves Expansion

For a radially symmetric potential, the Schrödinger equation (2.1) is rotationally invariant, but the boundary conditions (2.2) for the scattering wave function $\psi(\mathbf{r})$ are not. So ψ is not an eigenfunction of angular momentum, but it can be expanded in eigenfunctions of angular momentum. Since rotational symmetry around the z-axis is conserved both by the Schrödinger equation (2.1) and the boundary conditions (2.2), the azimuthal quantum number m is conserved. Since the incoming plane wave has $m = 0$, the same can be assumed for the full wave function $\psi(\mathbf{r})$, which thus no longer depends on the azimuthal angle ϕ,

$$\psi(\mathbf{r}) = \psi(r,\theta) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos\theta). \tag{2.33}$$

Equation (2.33) represents an expansion of the full scattering wave $\psi(\mathbf{r})$ in *partial waves*, each such partial wave being labelled by its orbital angular momentum quantum number l. The contribution of each partial wave is determined by its *radial wave function* $u_l(r)$. From the spherical representation of the Laplacian we have

$$-\frac{\hbar^2}{2\mu}\Delta = -\frac{\hbar^2}{2\mu}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{\hat{\mathbf{L}}^2}{2\mu r^2}, \tag{2.34}$$

and inserting the expansion (2.33) into the Schrödinger equation (2.1) leads to the equations

$$\left[-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)\hbar^2}{2\mu r^2}+V(r)\right]u_l(r)=Eu_l(r) \tag{2.35}$$

for the radial wave functions $u_l(r)$. The $1/r$ on the right-hand side of (2.33) ensures that the *radial Schrödinger equation* (2.35) contains only the second and not the first derivative of u_l, so it has the form of a Schrödinger equation for a particle moving in one dimension under the influence of the effective potential

$$V_{\mathrm{eff}}(r)=V(r)+V_{\mathrm{cent}}(r),\quad V_{\mathrm{cent}}(r)=\frac{l(l+1)\hbar^2}{2\mu r^2}, \tag{2.36}$$

subject to the condition that the coordinate r is nonnegative, $r\geq 0$. In the space of all possible radial wave functions in the lth partial wave, the unitary scalar product of two radial wave functions, u_l and $\tilde{u}_l$ is defined as

$$\langle u_l|\tilde{u}_l\rangle=\int_0^\infty u_l(r)^*\tilde{u}_l(r)\mathrm{d}r. \tag{2.37}$$

The effective potential (2.36) is essentially the same as in the classical description, see Eq. (1.11) in Sect. 1.2, except that the square of the angular momentum in the centrifugal potential is expressed via its quantum mechanical eigenvalue $l(l+1)\hbar^2$.

2.3.3 Scattering Phase Shifts

In the absence of the potential $V(r)$, the radial Schrödinger equation (2.35) represents the angular momentum components of the free-particle wave equation, and its solutions can be written as functions of the dimensionless product kr. Two linearly independent solutions of the radial free-particle equation are,

$$u_l^{(\mathrm{s})}(kr)=krj_l(kr),\qquad u_l^{(\mathrm{c})}(kr)=-kry_l(kr), \tag{2.38}$$

where j_l and y_l stand for the *spherical Bessel functions* of the first and second kind, respectively (see Appendix B.4 and Ref. [1]). Their asymptotic behaviour is given by

$$\begin{aligned} u_l^{(\mathrm{s})}(kr)&\overset{kr\to\infty}{=}\sin\left(kr-l\frac{\pi}{2}\right)+O\left(\frac{1}{kr}\right),\\ u_l^{(\mathrm{c})}(kr)&\overset{kr\to\infty}{=}\cos\left(kr-l\frac{\pi}{2}\right)+O\left(\frac{1}{kr}\right). \end{aligned} \tag{2.39}$$

For small values of kr, the radial free-particle wave functions (2.38) behave as,

$$\begin{aligned} u_l^{(\mathrm{s})}(kr) &\overset{kr\to 0}{\sim} \frac{\sqrt{\pi}(kr)^{l+1}}{2^{l+1}\Gamma(l+\frac{3}{2})}\left[1-\frac{(kr)^2}{4l+6}\right], \\ u_l^{(\mathrm{c})}(kr) &\overset{kr\to 0}{\sim} \frac{2^l\Gamma(l+\frac{1}{2})}{\sqrt{\pi}(kr)^l}\left[1+\frac{(kr)^2}{4l-2}\right]. \end{aligned} \tag{2.40}$$

The wave function $u_l^{(\mathrm{s})}$ is the physical, *regular* solution; $u_l^{(\mathrm{c})}$ is an unphysical, *irregular* solution. For $l>0$, the irregular solution $u_l^{(\mathrm{c})}$ is not square integrable due to the divergence at $r\to 0$; for $l=0$ its contribution proportional to $1/r$ in the full wave function (2.33) would lead to a delta-function contribution in $\Delta\psi$, which cannot be compensated by any other term in the Schrödinger equation (2.1).

For a potential $V(r)$ less singular than $1/r^2$ at the origin, the effective potential (2.36) is dominated near $r=0$ by the centrifugal term, so we can expect two linearly independent solutions of (2.35), u_l^{reg} and $u_l^{\mathrm{irr}}(r)$, whose small-distance behaviour is

$$u_l^{\mathrm{reg}}(r) \overset{r\to 0}{\propto} r^{l+1}, \qquad u_l^{\mathrm{irr}}(r) \overset{r\to 0}{\propto} r^{-l}. \tag{2.41}$$

Here u_l^{reg} denotes the physical, regular solution; u_l^{irr} is an unphysical, irregular solution. In the following, we shall mostly be dealing with regular solutions of the radial Schrödinger equation, which vanish for $r\to 0$, and we shall dispense with the superscript "reg" unless it is explicitly needed.

At large distances, the effective potential (2.36) is again dominated by the centrifugal term, because we have assumed that $V(r)$ falls off faster than $1/r^2$. The regular solution of the radial Schrödinger equation (2.35) can, at large distances, be taken to be a superposition of the two radial free-particle wave functions (2.38) obeying (2.39),

$$u_l(r) \overset{r\to\infty}{\propto} Au_l^{(\mathrm{s})}(kr) + Bu_l^{(\mathrm{c})}(kr) \overset{r\to\infty}{\propto} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right), \tag{2.42}$$

with $\tan\delta_l = B/A$. Since the potential is real, we can assume that u_l is, except for a constant complex factor, a real function of r, so that the ratio B/A and the phase δ_l are real. The phases δ_l, $l=0,1,2,\ldots$, contain the information about the effect of the potential on the asymptotic behaviour of the wave function (2.33). They are called *scattering phase shifts*, because they determine the scattering amplitude, as shown in the following.

The partial-waves expansion of the incoming plane wave is

$$\mathrm{e}^{\mathrm{i}kz} = \sum_{l=0}^{\infty}(2l+1)\mathrm{i}^l j_l(kr)P_l(\cos\theta), \tag{2.43}$$

where the j_l are the spherical Bessel functions of the first kind, already introduced in Eq. (2.38). At large distances, the full wave function consists of the plane wave

(2.43) and an outgoing spherical wave according to (2.2). The scattering amplitude f depends only on the polar angle θ, because the whole wave function does not depend on the azimuthal angle ϕ. We expand f into partial-wave contributions,

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos\theta), \tag{2.44}$$

with constant coefficients f_l, the *partial-wave scattering amplitudes*. Expressing the sum of plane and spherical wave in the form (2.33) gives an explicit expression for the asymptotic behaviour of the radial wave functions,

$$\begin{aligned} u_l(r) &\overset{r\to\infty}{\sim} \mathrm{i}^l\left[\frac{2l+1}{k}\sin\left(kr - l\frac{\pi}{2}\right) + f_l \mathrm{e}^{\mathrm{i}(kr - l\pi/2)}\right] \\ &= \mathrm{i}^l\left[\left(\frac{2l+1}{k} + \mathrm{i}f_l\right)\sin\left(kr - l\frac{\pi}{2}\right) + f_l\cos\left(kr - l\frac{\pi}{2}\right)\right]. \end{aligned} \tag{2.45}$$

Comparing Eqs. (2.45) and (2.42) shows that the coefficients of the sine and cosine terms in the square bracket in the lower line of (2.45) can be interpreted as the coefficients A and B in (2.42), for which $\tan\delta_l = B/A$. With the coefficients in (2.45),

$$\cot\delta_l = \frac{A}{B} \equiv \frac{2l+1}{kf_l} + \mathrm{i} \quad \Rightarrow \quad \cot\delta_l - \mathrm{i} = \frac{\mathrm{e}^{-\mathrm{i}\delta_l}}{\sin\delta_l} = \frac{2l+1}{kf_l}, \tag{2.46}$$

which leads to

$$f_l = \frac{2l+1}{k}\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l = \frac{2l+1}{2\mathrm{i}k}\left(\mathrm{e}^{2\mathrm{i}\delta_l} - 1\right). \tag{2.47}$$

With (2.45) the asymptotic form of the radial wave functions is,

$$u_l(r) \overset{r\to\infty}{\sim} \frac{2l+1}{k}\mathrm{i}^l\mathrm{e}^{\mathrm{i}\delta_l}\sin\left(kr - l\frac{\pi}{2} + \delta_l\right), \tag{2.48}$$

and the asymptotic form of the full wave function (2.33) is

$$\psi(\mathbf{r}) \overset{r\to\infty}{\sim} \sum_{l=0}^{\infty}\frac{2l+1}{kr}\mathrm{i}^l\mathrm{e}^{\mathrm{i}\delta_l}\sin\left(kr - l\frac{\pi}{2} + \delta_l\right)P_l(\cos\theta). \tag{2.49}$$

The explicit expression, (2.44) with (2.47), for the scattering amplitude allows us to express the differential scattering cross section in terms of the scattering phase shifts δ_l,

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left|f(\theta)\right|^2 = \frac{1}{k^2}\sum_{l,l'}\mathrm{e}^{\mathrm{i}(\delta_l - \delta_{l'})}(2l+1)\sin\delta_l\left(2l'+1\right)\sin\delta_{l'}P_l(\cos\theta)P_{l'}(\cos\theta). \tag{2.50}$$

For the integrated scattering cross section we can exploit the orthogonality (2.30) of the Legendre polynomials,

$$\sigma = \sum_{l=0}^{\infty} \frac{4\pi}{2l+1} |f_l|^2 = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2 \delta_l = \frac{\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \left| e^{2i\delta_l} - 1 \right|^2. \quad (2.51)$$

The integrated scattering cross section is the incoherent sum of the contributions $\sigma_{[l]}$,

$$\sigma = \sum_{l=0}^{\infty} \sigma_{[l]}, \quad \sigma_{[l]} = \frac{4\pi}{k^2} (2l+1) \sin^2 \delta_l. \quad (2.52)$$

The maximum contribution of a given partial wave l to the integrated cross section is realized when δ_l is an odd multiple of $\frac{\pi}{2}$, so $\sin^2 \delta_l = 1$,

$$(\sigma_{[l]})_{\max} = \frac{4\pi}{k^2} (2l+1). \quad (2.53)$$

2.3.4 Normalization of Radial Wave Functions

A radial wave function $u_b(r)$ describing a negative-energy bound state in a given partial wave l is square-integrable and can be normalized to unity,

$$\langle u_b | u_b \rangle = \int_0^{\infty} u_b(r)^* u_b(r) dr = 1. \quad (2.54)$$

The regular solutions $u_l^{(k)}(r)$ of the radial Schrödinger equation at positive energies, $E = \hbar^2 k^2/(2\mu)$ $[k > 0]$, are orthogonal,

$$\left\langle u_l^{(k)} \middle| u_l^{(k')} \right\rangle = \int_0^{\infty} u_l^{(k)}(r)^* u_l^{(k')}(r) dr = 0 \quad \text{for } k \neq k', \quad (2.55)$$

but the integral diverges for $k = k'$, because the integrand is asymptotically proportional to $\sin^2(kr - \frac{\pi}{2} l + \delta_l)$. We can write

$$\left\langle u_l^{(k)} \middle| u_l^{(k')} \right\rangle \propto \delta(k - k'), \quad (2.56)$$

but this relation is not so useful as long as the proportionality constant is not known.

For pure sine waves of unit amplitude, $u_s^{(k)} = \sin(kr)$ $[k > 0]$, it is easy to see that

$$\left\langle u_s^{(k)} \middle| u_s^{(k')} \right\rangle = \int_0^{\infty} \sin(kr) \sin(k'r) dr = \frac{\pi}{2} \delta(k - k'). \quad (2.57)$$

The right-hand side of Eq. (2.57) remains unchanged, if we replace the wave functions $u_s^{(k)}$ by regular solutions of the radial Schrödinger equation which behave

asymptotically as $\sin(kr - \frac{\pi}{2}l + \delta_l)$. For $k \neq k'$ this follows according to (2.55). For $k = k'$ we can divide the integral from $r = 0$ to $r = \infty$ into a finite integral from $r = 0$ to some arbitrarily large but finite radius r_{large}, and an integral from r_{large} to $r = \infty$, which is the infinite part that determines the prefactor of the delta function. In the latter integral, the radial wave function is well described by the sine with unit amplitude, and the shift of argument, $-\frac{\pi}{2}l + \delta_l$, does not affect the result. We can thus define regular radial wave functions that are *normalized in wave number* as follows:

$$u_l^{(k)}(r) \overset{r\to\infty}{\sim} \sqrt{\frac{2}{\pi}} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right) \quad \Longrightarrow \quad \left\langle u_l^{(k)} \middle| u_l^{(k')} \right\rangle = \delta\big(k - k'\big). \tag{2.58}$$

The identity

$$\delta\big(k - k'\big) = \frac{\mathrm{d}E}{\mathrm{d}k}\delta\big(E - E'\big) = \frac{\hbar^2 k}{\mu}\delta\big(E - E'\big) \tag{2.59}$$

leads to the appropriate definition of the regular radial wave functions $\bar{\mathrm{u}}_l^{(E)}$, which are *normalized in energy*,

$$\bar{\mathrm{u}}_l^{(E)}(r) \overset{r\to\infty}{\sim} \sqrt{\frac{2\mu}{\pi\hbar^2 k}} \sin\left(kr - l\frac{\pi}{2} + \delta_l\right) \quad \Longrightarrow \quad \left\langle \bar{\mathrm{u}}_l^{(E)} \middle| \bar{\mathrm{u}}_l^{(E')} \right\rangle = \delta\big(E - E'\big). \tag{2.60}$$

2.3.5 Radial Lippmann–Schwinger Equation

The radial Schrödinger equation (2.35) can be rewritten as

$$\left[E + \frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right] u_l(r) = V(r)u_l(r) \tag{2.61}$$

and transformed into an integral equation with the help of the *radial free-particle Green's function* $\mathscr{G}_l(r, r')$, which fulfills

$$\left[E + \frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l(l+1)\hbar^2}{2\mu r^2}\right] \mathscr{G}_l\big(r, r'\big) = \delta\big(r - r'\big) \tag{2.62}$$

and is explicitly given by

$$\mathscr{G}_l\big(r, r'\big) = -\frac{2\mu}{\hbar^2 k} u_l^{(\mathrm{s})}(kr_<) u_l^{(\mathrm{c})}(kr_>); \tag{2.63}$$

here $u_l^{(\mathrm{s})}$ and $u_l^{(\mathrm{c})}$ stand for the regular and irregular free-particle radial waves as defined in (2.38), and $r_<$ stands for the smaller while $r_>$ stands for the larger of the

two radial coordinates r and r'. A wave function obeying the integral equation

$$u_l(r) = u_l^{(\mathrm{s})}(kr) + \int_0^\infty \mathscr{G}_l(r, r')\, V(r')\, u_l(r') \tag{2.64}$$

necessarily obeys the radial Schrödinger equation (2.61). This would also hold if the first term $u_l^{(\mathrm{s})}(kr)$ were replaced by any other solution of the "homogeneous" version $[E + \cdots]u_l(r) = 0$ of Eq. (2.61).[3]

Equation (2.64) is the *radial Lippmann–Schwinger equation* in the lth partial wave. Asymptotically, $r \to \infty$, we can assume $r = r_>$ and $r' = r_<$ in the radial Green's function, so the factor $u_l^{(\mathrm{c})}(kr_>) = u_l^{(\mathrm{c})}(kr)$ can be drawn out of the integral over r',

$$u_l(r) \overset{r\to\infty}{\sim} u_l^{(\mathrm{s})}(kr) - \left[\frac{2\mu}{\hbar^2 k}\int_0^\infty u_l^{(\mathrm{s})}(kr')\, V(r')\, u_l(r')\,\mathrm{d}r'\right] u_l^{(\mathrm{c})}(kr). \tag{2.65}$$

Comparing with Eq. (2.42) shows that the coefficient of $u_l^{(\mathrm{c})}(kr)$ in (2.65) is the tangent of the scattering phase shift,

$$\tan\delta_l = -\frac{2\mu}{\hbar^2 k}\int_0^\infty u_l^{(\mathrm{s})}(kr)\, V(r)\, u_l(r)\,\mathrm{d}r. \tag{2.66}$$

The expression on the right-hand side of (2.66) cannot be evaluated explicitly, because it still contains the (usually unknown) exact solution u_l of the radial Schrödinger equation. It does, however, offer a possibility for approximation in the spirit of the Born approximation. Replacing $u_l(r)$ in the integrand in (2.66) by the regular free-particle radial wave $u_l^{(\mathrm{s})}(kr)$ gives an explicit but approximate expression for $\tan\delta_l$, in the spirit of the first-order Born approximation:

$$\tan\delta_l^{\mathrm{Born}} = -\frac{2\mu}{\hbar^2 k}\int_0^\infty \left[u_l^{(\mathrm{s})}(kr)\right]^2 V(r)\,\mathrm{d}r. \tag{2.67}$$

Note that the right-hand side of (2.67) is a smooth function of k that always remains finite. Hence δ_l^{Born} as function of k can never cross an odd multiple of $\frac{\pi}{2}$. Equation (2.67) can only be a useful approximation when the phase shifts are restricted to a small interval around zero (or an integer multiple of π); for potentials which are bounded and short ranged, this happens both in the limit of high energies and in the limit of large angular momentum quantum numbers l, see Sect. 2.6.4.

[3] See footnote in Sect. 2.2.

2.3.6 S-Matrix

The asymptotic behaviour of the radial wave function (2.48) can be written as

$$u_l(r) \overset{r\to 0}{\sim} \frac{2l+1}{2k} \mathrm{i}^{l+1} \left[\mathrm{e}^{-\mathrm{i}(kr - l\pi/2)} - \mathrm{e}^{2\mathrm{i}\delta_l} \mathrm{e}^{+\mathrm{i}(kr - l\pi/2)} \right]$$
$$= \frac{2l+1}{2k} \mathrm{i}^{2l+1} \left[\mathrm{e}^{-\mathrm{i}kr} - (-1)^l \mathrm{e}^{2\mathrm{i}\delta_l} \mathrm{e}^{+\mathrm{i}kr} \right]. \tag{2.68}$$

In both lines of (2.68), the square bracket contains an incoming radial wave proportional to $\mathrm{e}^{-\mathrm{i}kr\cdots}$ and an outgoing radial wave proportional to $\mathrm{e}^{+\mathrm{i}kr\cdots}$. The factor $\mathrm{e}^{2\mathrm{i}\delta_l}$ in the outgoing wave is the contribution of the lth partial wave to the *scattering matrix* or S-matrix,

$$S_l = \mathrm{e}^{2\mathrm{i}\delta_l}. \tag{2.69}$$

For the radial potential $V(r)$, the S-matrix is diagonal, because there is no coupling between the radial Schrödinger equations (2.35) of different l.

The S-matrix is *unitary*, which, for the partial-wave contribution (2.69) means $|S_l| = 1$. This is an expression of particle conservation and is fulfilled as long as the scattering phase shifts δ_l are real. Equation (2.53) is based on the assumption, that the phase shifts are real, i.e., that the S-matrix is unitary. Its right-hand side $(4\pi/k^2)(2l+1)$ is hence called the *unitarity limit* of the contribution of the respective partial wave to the integrated scattering cross section.

For real δ_l, the scattering amplitude (2.44) with the partial-wave amplitudes (2.47) can be decomposed into real and imaginary parts as follows:

$$f(\theta) = \sum_{l=0}^{\infty} \frac{2l+1}{k} \left[\cos\delta_l \sin\delta_l + \mathrm{i}\sin^2\delta_l \right] P_l(\cos\theta). \tag{2.70}$$

For the forward direction, $\theta = 0$, we insert $P_l(1) = 1$ and recall Eq. (2.51),

$$\Im\left[f(\theta=0)\right] = \sum_{l=0}^{\infty} \frac{2l+1}{k} \sin^2\delta_l = \frac{k}{4\pi}\sigma, \tag{2.71}$$

thus recovering the optical theorem (2.14). The unitarity of the S-matrix is an expression of particle conservation. Note that the radial Born approximation (2.67) yields real phase shifts and a unitary S-matrix, so it is compatible with particle conservation. This is in contrast to the Born approximation (2.22) for the scattering amplitude. For a radially symmetric potential V, the Born scattering amplitude (2.22) is a real function of the modulus of the momentum transfer vector (2.23) and necessarily violates the optical theorem.

2.3.7 Determination of the Scattering Phase Shifts

The boundary condition $u_l(r) \overset{r\to 0}{\propto} r^{l+1}$ uniquely determines the radial wave function except for a constant factor. The scattering phase shifts δ_l can be calculated by integrating the radial Schrödinger equation (2.35) with this boundary condition from small r to a finite radius r_m, where the potential $V(r)$ has already fallen off sufficiently to be negligible. Matching the logarithmic derivative u_l'/u_l to the logarithmic derivative of a superposition (2.42) of the free-particle wave functions at $r = r_\mathrm{m}$ yields $\tan\delta_l$.

Due to the influence of the potential at short distances, the nodes (beyond $r = 0$) and antinodes of the radial wave function $u_l(r)$ are shifted relative to those of the regular free-particle wave function $u_l^{(\mathrm{s})}$. This leads to asymptotic *spatial shifts* d_l, which are related to the phase shifts δ_l by $d_l = \delta_l/k$, as can be seen by writing u_l as

$$u_l(r) \overset{r\to\infty}{\propto} \sin\left[k\left(r + \frac{\delta_l}{k}\right) - l\frac{\pi}{2}\right]. \tag{2.72}$$

For a repulsive potential V, the radial wave function is suppressed at small distances and its nodes (beyond $r = 0$) and antinodes are pushed to larger values of r by the potential; the spatial shifts, and hence also the phase shifts, are negative. The simplest example is scattering by a hard sphere of radius R. For $r > R$, the potential vanishes, and the radial wave function can be written as $Au_l^{(\mathrm{s})}(kr) + Bu_l^{(\mathrm{c})}(kr)$, see Eq. (2.42). The wave function must vanish for $r \le R$, so the inner boundary condition is pushed out from $r = 0$ to $r = R$. The condition $Au_l^{(\mathrm{s})}(kR) + Bu_l^{(\mathrm{c})}(kR) = 0$ yields

$$\frac{B}{A} = -\frac{u_l^{(\mathrm{s})}(kR)}{u_l^{(\mathrm{c})}(kR)} = \frac{j_l(kR)}{y_l(kR)}, \qquad \delta_l = \arctan\left(\frac{j_l(kR)}{y_l(kR)}\right). \tag{2.73}$$

From (2.40) and (2.39), the low- and high-energy behaviour of the hard-sphere phase shifts is

$$\begin{aligned} \delta_l &\overset{kR\to 0}{\sim} -\frac{\pi}{\Gamma(l+\frac{3}{2})\Gamma(l+\frac{1}{2})}\left(\frac{kR}{2}\right)^{2l+1}\left[1 - \left(\frac{kR}{2}\right)^2\left(\frac{1}{l-\frac{1}{2}} + \frac{1}{l+\frac{3}{2}}\right)\right], \\ \delta_l &\overset{kR\to\infty}{\sim} -kR + l\frac{\pi}{2} \end{aligned} \tag{2.74}$$

for $l > 0$, while $\delta_{l=0} = -kR$ for all k. Note that the high-energy behaviour in the lower line of (2.74) implies that the radial wave function (2.72) has the same asymptotic behaviour in all partial waves in the high-energy limit,

$$u_l(r) \overset{r\to\infty, kR\to\infty}{\propto} \sin(kr - kR). \tag{2.75}$$

This is because, for any angular momentum l, the radial classical turning point always reaches the radius R of the hard sphere at a sufficiently high energy, and the

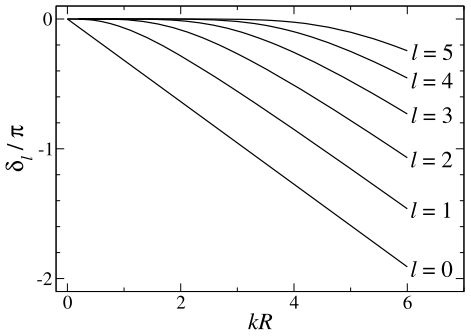

Fig. 2.3 Scattering phase shifts (2.73) for scattering by a hard sphere of radius R

influence of the centrifugal potential diminishes continuously as the energy rises further above this value. The phase shifts (2.73) for scattering by a hard sphere are shown in Fig. 2.3 for partial waves from $l = 0$ to $l = 5$.

For an attractive potential, the oscillations are of smaller wavelength in the interaction region and a given node (beyond $r = 0$) or antinode is pulled in to shorter distances by the potential; the spatial shift and the phase shift are positive. The behaviour of the phase shift depends on whether the effective potential features an attractive well that is deep enough to support one or more bound states, and the near-threshold behaviour of the phase shift depends sensitively on whether or not there is a bound state close to threshold.

2.3.8 *Near-Threshold Behaviour of the Scattering Phase Shifts*

The leading near-threshold behaviour of the phase shifts can be derived from the small-argument behaviour of the free-particle solutions. At distances r beyond the range of the potential, the radial wave function $u_l(r)$ is a superposition of the free-particle wave functions (2.38); towards threshold, $k \to 0$, the product kr tends to zero so we can make use of the small-argument expressions (2.40),

$$\begin{aligned} u_l(r) &\overset{kr\to 0}{\propto} u_l^{(\mathrm{s})}(kr) + \tan\delta_l u_l^{(\mathrm{c})}(kr) \\ &\sim \frac{\sqrt{\pi}k^{l+1}}{2^{l+1}\Gamma(l+\frac{3}{2})}\left[r^{l+1} + \tan\delta_l \frac{2^{2l+1}\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}{\pi k^{2l+1} r^l}\right]. \end{aligned} \tag{2.76}$$

Directly at threshold, the radial Schrödinger equation (2.35) has a regular solution $u_l^{(0)}(r)$ which is defined up to a constant by the boundary condition $u_l^{(0)}(0) = 0$ and is function of r only. The wave function (2.76) must become proportional to this

k-independent solution for $k \to 0$, so in the second term in the square bracket in the lower line of Eq. (2.76), the k-dependence of $\tan\delta_l$ must compensate the factor k^{2l+1} in the denominator, $\tan\delta \overset{k\to 0}{\propto} k^{2l+1}$. More explicitly,

$$\tan\delta_l \overset{k\to 0}{\sim} -\frac{\pi}{\Gamma(l+\frac{1}{2})\Gamma(l+\frac{3}{2})}\left(\frac{a_l k}{2}\right)^{2l+1}. \tag{2.77}$$

The characteristic length a_l appearing on the right-hand side of (2.77) is the *scattering length* in the lth partial wave.

The proportionality to k^{2l+1} in (2.77) expresses growing suppression with increasing l due to the influence of the centrifugal barrier separating the asymptotic region of free-particle motion from the interaction region at small distances. It is typical for the l-dependence of quantum mechanical quantities involving a centrifugal barrier and is generally referred to as *Wigner's threshold law*.

Equation (2.77) implies that the leading behaviour of the partial-wave scattering amplitude (2.47) is

$$f_l \overset{k\to 0}{\propto} k^{2l}, \tag{2.78}$$

which means that small l-values dominate the scattering amplitude (2.44) and the scattering cross sections (2.50), (2.51) at low energies. For s-waves, Eq. (2.77) reads

$$\tan\delta_0 \overset{k\to 0}{\sim} -ak, \tag{2.79}$$

where we have dropped the subscript on the a, as is customary. The s-wave scattering length a in (2.79) is generally referred to as *the* scattering length, a concept introduced by Fermi and Marshall in 1947 [15]. From (2.78) it follows that only the s-wave retains a nonvanishing contribution to the scattering amplitude (2.44) in the limit $k \to 0$,

$$\lim_{k\to 0} f(\theta) = f_0 P_0 \sim -a \quad \Longrightarrow \quad \lim_{k\to 0}\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = a^2 \quad \text{and} \quad \lim_{k\to 0}\sigma = 4\pi a^2. \tag{2.80}$$

For hard-sphere scattering, the scattering length is the radius of the sphere, and the threshold limit of the quantum mechanical integrated scattering cross section is $4\pi R^2$, which is four times the classical cross section, see Eq. (1.39) in Sect. 1.3.

The definition (2.79) of the scattering length for s-waves is universally accepted. For $l > 0$, the definitions of the scattering length vary. Some authors, e.g. [44], even call the whole coefficient of k^{2l+1} in (2.77) scattering length, although this coefficient has the physical dimension of a length to the power $2l+1$. The definition (2.77) ensures that a_l is a length and that for scattering by a hard sphere of radius R we have $a_l = R$ for all l, as can be seen by comparing with (2.74).

With (2.77), the threshold solution of the radial Schrödinger equation (2.35) behaves asymptotically as,

$$u_l^{(0)}(r) \overset{r\to\infty}{\propto} r^{l+1} - \frac{a_l^{2l+1}}{r^l}, \tag{2.81}$$

so the scattering length appears as the zero of the asymptotic behaviour of the threshold solution of the radial Schrödinger equation. The leading term in (2.81) is proportional to r^{l+1} and comes naturally by integrating outwards under the centrifugal potential. The proportionality of the next-to-leading term to r^{-l} is not so universal and is subject to conditions on the asymptotic fall-off of the potential $V(r)$. For a potential falling off asymptotically as an inverse power of r, $V(r) \overset{r\to\infty}{\propto} 1/r^{\alpha}$, $\alpha > 2$, the next-to-leading term is proportional to r^{-l} *only* if

$$\alpha > 2l + 3, \tag{2.82}$$

as is shown later in Sect. 2.6. The definition (2.77) of the partial-wave scattering length and the behaviour (2.81) of the threshold wave function apply only for potentials which fall off faster than $1/r^{2l+3}$ at large distances. The s-wave scattering length is well defined for potentials falling off faster than $1/r^3$, the p-wave ($l = 1$) scattering length for potentials falling off faster than $1/r^5$.

When the scattering length vanishes, the threshold solution (2.81) is asymptotically proportional to r^{l+1}, just as the regular solution of the radial Schrödinger equation for the centrifugal potential alone. An infinite scattering length, $|a_l| \to \infty$, implies that the threshold solution of the radial Schrödinger equation (2.35) decays as $1/r^l$ for large distances. For $l > 0$ this means that there is a normalizable wave function solving the radial Schrödinger equation at $E = 0$, i.e., a bound state exactly at threshold.

For s-waves, Eq. (2.81) reads

$$u_{l=0}^{(0)} \overset{r\to\infty}{\propto} r - a \propto 1 - \frac{r}{a}. \tag{2.83}$$

An infinite s-wave scattering length means that the threshold solution becomes constant at large distances. One speaks of a bound state at threshold in this case as well, even though the wave function is not normalizable.

The scattering length depends very sensitively on whether there is a bound state very close to threshold, or whether the potential just fails to bind a further bound state. This is easily demonstrated via the simple but instructive example of an attractive sharp-step potential,

$$V(r) = \begin{cases} -V_S & \text{for } r \le L, \\ 0 & \text{for } r > L, \end{cases} \qquad V_S = \frac{\hbar^2 K_S^2}{2\mu}. \tag{2.84}$$

When $K_S L = \frac{\pi}{2}$, which corresponds to a depth V_S equal to the energy $E_0 = (\frac{\pi}{2}\hbar)^2/(2\mu L^2)$, the potential (2.84) has a threshold solution which becomes constant for $r > L$. For a slightly deeper step, $V_S = 1.4E_0$, the potential supports a weakly bound state at the energy $E_b \approx -0.189E_0$, indicated by the horizontal dotted brown line in the left half of Fig. 2.4; the associated bound-state wave function is shown as dashed brown line. As is customary in such illustrations, the zero-axis for a wave function is chosen to lie at the energy for which it solves the Schrödinger equation. The threshold solution at $E = 0$ (solid blue line) is not very different

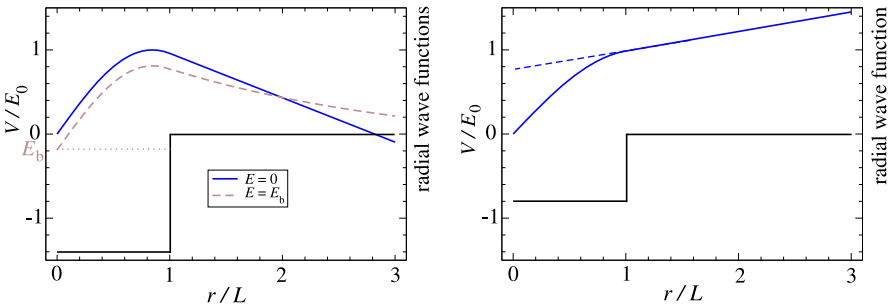

Fig. 2.4 Sharp-step potential (2.84). The energy is given in units of $E_0 = (\frac{\pi}{2}\hbar)^2/(2\mu L^2)$. For $V_S = E_0$, the s-wave radial Schrödinger equation has a zero-energy solution which becomes constant for $r \geq L$. The left half of the figure shows the case $V_S = 1.4E_0$, for which the potential supports a bound state at the energy $E_b \approx -0.189E_0$, indicated by the *horizontal dotted brown line*. The bound-state wave function is shown as *dashed brown line*, and its zero-axis lies at its energy E_b. The threshold solution is shown as *solid blue line* with zero-axis at $E = 0$; for $r > L$ it is a linear function which cuts the axis at a distance defining the scattering length a. The right half of the figure shows the case $V_S = 0.8E_0$, for which there is no bound state; the threshold solution (*solid blue line*) is a straight line for $r > L$, and the extrapolation of this line to smaller r-values leads to an intersection with the r-axis at a large negative value, corresponding to a large negative scattering length a

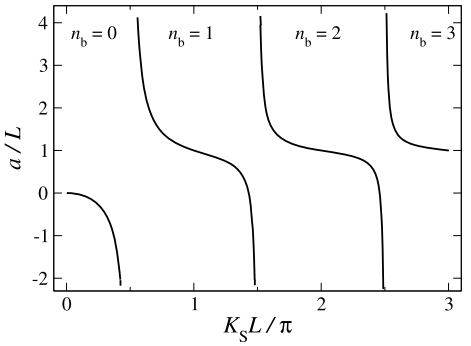

Fig. 2.5 Scattering length for the sharp-step potential as function of the threshold wave number K_S, as given by Eq. (2.85). Each pole indicates the existence of a bound state at threshold; n_b is the number of bound states supported by the potential for values of K_S between successive poles

from the bound-state wave function for $r \leq L$. For $r > L$ the potential vanishes, so the threshold solution assumes its asymptotic behaviour (2.83) corresponding to a linear fall-off; it cuts the r-axis at a value defining the scattering length a ($\approx 2.8L$ in the present case). The right half of Fig. 2.4 shows a shallower step, $V_S = 0.8E_0$, for which the potential just fails to support a bound state. The threshold solution (solid blue line) now *grows* linearly for $r > L$. Extrapolation of this linear behaviour to smaller r-values eventually leads to a crossing of the r-axis at a large negative value, corresponding to a large negative scattering length. The dependence of the scattering length on the potential depth V_S, or on the related threshold wave number $K_S = \sqrt{2\mu V_S}/\hbar$, can be easily deduced from the threshold solution $u^{(0)}_{l=0}(r) \overset{r \leq L}{\propto} \sin(K_S r)$. Its logarithmic derivative at $r = L$ is $K_S \cot(K_S L)$ which

must be equal to $1/(L-a)$ according to (2.83), so [24]

$$a = L - \frac{\tan(K_S L)}{K_S}. \tag{2.85}$$

Figure 2.5 shows the behaviour of the scattering length as function of the threshold wave number K_S. It is typical for the behaviour of the scattering length of a potential as function of a parameter which can tune the number and positions of bound states in the potential. The scattering length has a pole whenever there is a bound state at threshold. Before the first pole ($K_S L < 0.5\pi$ in Fig. 2.5), the potential has no bound states. The number of bound states increases by one every time K_S increases through a pole.

A quantitative relation between the diverging scattering length and the vanishing eigenenergy of a near-threshold bound state can be derived quite generally as follows: Assume that there is a bound s-state at an energy $E_b = -\hbar^2\kappa_b^2/(2\mu)$ very close to threshold. Beyond the range of the potential, the radial wave function $u_{l=0}^{(\kappa_b)}$ at this energy is proportional to $e^{-\kappa_b r}$ and behaves as

$$u_{l=0}^{(\kappa_b)}(r) \propto 1 - r\left[\kappa_b + O\left(\kappa_b^2\right)\right] \quad (\kappa_b < 0). \tag{2.86}$$

The terms below order κ_b^2 in (2.86) are compatible with (2.83) if we assume

$$\frac{1}{a} \overset{\kappa_b \to 0}{\sim} \kappa_b + O\left(\kappa_b^2\right). \tag{2.87}$$

This is plausible, since the radial Schrödinger equation at energy E_b differs from the radial Schrödinger equation at threshold by a term of order κ_b^2. Equation (2.87) implies the following relation between the scattering length a and the inverse penetration depth κ_b of a bound state very near threshold,

$$a \overset{\kappa_b \to 0}{\sim} \frac{1}{\kappa_b} + O\left(\kappa_b^0\right). \tag{2.88}$$

Conversely, a large positive scattering length a implies a near-threshold bound state, whose energy is given by,

$$E_b = -\frac{\hbar^2\kappa_b^2}{2\mu} \overset{a \to \infty}{\sim} -\frac{\hbar^2}{2\mu a^2} + O\left(\frac{1}{a^3}\right). \tag{2.89}$$

When the potential just fails to bind a further bound state, there may be a solution $u_{l=0}^{v}$ of the s-wave radial Schrödinger equation which is asymptotically proportional to $e^{+\kappa_v r}$ with a very small positive κ_v. By the same arguments as above, such a solution of (2.35) gives rise to a large negative scattering length, $a \overset{\kappa_v \to 0}{\sim} -1/\kappa_v + O(\kappa_v^0)$. In such a situation one speaks of a *virtual state* at the energy $E_v = -\hbar^2\kappa_v^2/(2\mu)$ [33, 44].

The unambiguous identification of a virtual state poses a problem. The discrete energy of a genuine bound state is easily found via the condition that the wave

function must decay to zero as $e^{-\kappa r}$ at large distances. When solving the radial Schrödinger equation, e.g. by integrating it from smaller to larger r-values, any contribution from the exponentially growing solution soon becomes dominant and indicates that the energy under consideration is not a bound-state eigenvalue. On the other hand, the solution proportional to $e^{+\kappa r}$ cannot be unambiguously defined, unless the potential vanishes exactly after some finite, preferably short, distance. Any contribution of the solution proportional to $e^{-\kappa r}$ is soon dominated by the exponentially growing term, so it is very difficult in practice to decide, whether the contribution of the decaying solution vanishes exactly or not. This problem is aggravated as κ increases, so the concept of virtual states is most useful very close to threshold.

For a potential which falls off sufficiently rapidly at large distances, the next-to-leading behaviour of the scattering phase shifts near threshold, following the leading term (2.77), can be derived from solutions of the radial Schrödinger equation at threshold [3]. This is shown below for s-waves, $l = 0$. We shall drop the subscript $l = 0$, but remember that we are dealing with s-waves.

Let $u^{(0)}$ and $u^{(k)}$ be regular radial wave functions that solve the radial Schrödinger equation at threshold and for wave number $k > 0$,

$$\frac{\mathrm{d}^2 u^{(0)}}{\mathrm{d}r^2} = \frac{2\mu}{\hbar^2} V(r) u^{(0)}(r), \qquad \frac{\mathrm{d}^2 u^{(k)}}{\mathrm{d}r^2} = \left(\frac{2\mu}{\hbar^2} V(r) - k^2 \right) u^{(k)}(r). \tag{2.90}$$

There are two alternative representations for the integral

$$I_u(r_0) = \int_0^{r_0} \left[u^{(0)}(r) \frac{\mathrm{d}^2 u^{(k)}}{\mathrm{d}r^2} - u^{(k)}(r) \frac{\mathrm{d}^2 u^{(0)}}{\mathrm{d}r^2} \right] \mathrm{d}r. \tag{2.91}$$

One involves multiplying the first of the two equations (2.90) by $u^{(k)}$, the second by $u^{(0)}$, and integrating the difference; this leads to

$$I_u(r_0) = -k^2 \int_0^{r_0} u^{(0)}(r) u^{(k)}(r) \mathrm{d}r. \tag{2.92}$$

An alternative representation of the integral (2.91) is obtained by partial integration,

$$I_u(r_0) = \left[u^{(0)}(r) \frac{\mathrm{d}u^{(k)}}{\mathrm{d}r} - u^{(k)}(r) \frac{\mathrm{d}u^{(0)}}{\mathrm{d}r} \right]_0^{r_0} = u^{(0)}(r_0) \left. \frac{\mathrm{d}u^{(k)}}{\mathrm{d}r} \right|_{r_0} - u^{(k)}(r_0) \left. \frac{\mathrm{d}u^{(0)}}{\mathrm{d}r} \right|_{r_0}. \tag{2.93}$$

Contributions from the lower limit of integration, $r = 0$, vanish, because the regular solutions $u(r)$ vanish for $r \to 0$.

We now repeat the procedure for two (not necessarily regular) radial wave functions, $w^{(0)}$ and $w^{(k)}$, which solve the *free-particle* radial Schrödinger equation at threshold and for wave number $k > 0$,

$$\frac{\mathrm{d}^2 w^{(0)}}{\mathrm{d}r^2} = 0, \qquad \frac{\mathrm{d}^2 w^{(k)}}{\mathrm{d}r^2} = -k^2 w^{(k)}(r). \tag{2.94}$$

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