Week 6

PHY 304 Quantum Mechanics-II
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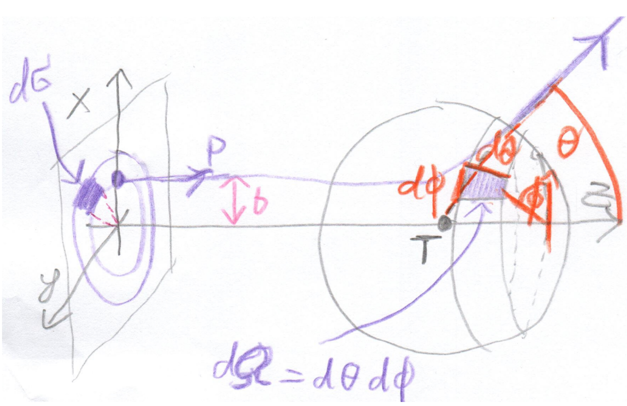
8 Quantum scattering theory

We had seen our first 1D example of quantum scattering with the square barrier problem in section 2.2.4. There the scattering had only two possible outcomes, transmission or reflection, which we could study as a function of only one parameter, the energy of the incoming particle. Most real life scattering events happen in 3D, we thus get a continuous range of outcomes namely two scattering angles θ, φ, as discussed shortly. We can also vary at least one more property of the incoming particle, the impact parameter.

8.1 Classical scattering theory

All concepts just mentioned are not special to quantum scattering theory, so we first briefly discuss (or review) scattering in classical mechanics.

The basic problem of scattering theory is sketched below. A projectile P is impacting on a target T with impact parameter b. The impact parameter is the distance to a straight line directly hitting the target. Typically the problem is azimuthally symmetric, independent of ϕ. The task is then to calculate the scattering angle θ (the deflection angle of the projectile from its incoming direction), as a function of the impact parameter and the energy (or momentum) of the incoming particle. This deflection will be due to some interaction between projectile and target, which in the sketch we have drawn as a long ranged, repulsive interaction, but the problem statement covers all interaction.



left: Geometry of a scattering event. We define the z-axis as going through the target and then parallel to the momentum of the projectile. Since the projectile might not move head-on towards the target, we offset its initial trajectory (violet) by the impact parameter b. We also sketch the angles θ, ϕ of the outgoing trajectory, in a spherical polar coordinate system centered on the target. The areas $d\sigma$ and $d\Omega$ (violet) are discussed further below.

By solving Newton's equation, we can predict θ for all possible incoming impact parameters and angles ϕ. Assuming the typical case where the interaction potential $V(|\mathbf{x}_P - \mathbf{x}_T|)$ between projectile and target only depends on their separation $r = |\mathbf{x}_P - \mathbf{x}_T|$, the problem is clearly azimuthally symmetric and the answer will not depend on ϕ. Let us define that all particles coming in through an (infinitesimal) cross sectional area $d\sigma$, will be scattered into a solid angle $d\Omega = d\theta d\phi$ (to be determined). We define the constant of proportionality $D(\theta)$ between the two as differential scattering cross-section

$$d\sigma = D(\theta) d\Omega. \tag{8.1}$$

Essentially it tells us "how likely a scattering event with deflection angle θ will be". Looking at the violet shades in the diagram above, we can deduce infinitesimal areas $d\sigma = b\, db\, d\phi$ and $d\Omega = \sin\theta\, d\theta\, d\phi$, which results in the following expression for the differential cross section

$$D(\theta) = \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|. \tag{8.2}$$

Let us collect all the quantities we defined above into a red box:

Quantities describing a scattering process For an impact parameter b and scattering angle θ we define a differential scattering cross-section

$$D(\theta) = \frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta} \left| \frac{db}{d\theta} \right|. \tag{8.3}$$

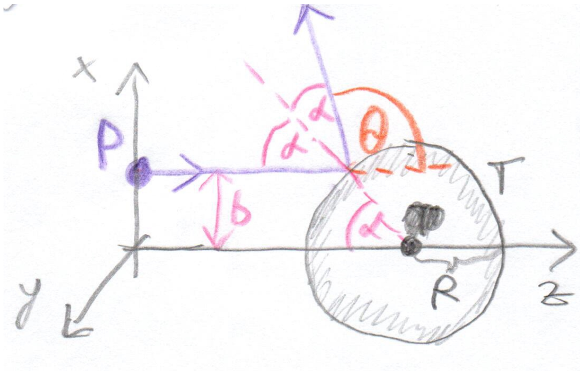
and from that a total scattering cross-section

$$\sigma = \int d\Omega D(\theta) \tag{8.4}$$

- See Eq. (4.49) for the definition of $\int d\Omega$.
- The total scattering cross section determines which segment of the incoming beam cross section is going to be deflected by the projectile (for very large b and a finite range of $V(r)$, this segment typically has a finite size).

It is best to see how all this work, by looking at an example (taken from Griffith)

Example 63, Classical scattering off a hard sphere: Imagine a small pebble being shot at a billiard ball of radius R and elastically reflecting off its surface as shown below.



left: Knowing the impact pararameter b, we can infer the angle α defined in the drawing as $\sin\alpha = b/R$, and then read off the drawing that the scattering angle is $\theta = \pi - 2\alpha$. Thus $b = R\sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) = R\cos\theta$ and hence

$$\theta = \begin{cases} 2\arccos(b/R) & \text{for } b < R \\ 0 & \text{for } b \geq R \end{cases} \tag{8.5}$$

To calculate the differential cross-section $D(\theta)$, we need $db/d\theta = -R\sin(\theta/2)/2$ from which we can find

$$D(\theta) = \frac{R\cos(\theta/2)}{\sin\theta}\frac{R\sin(\theta/2)}{2} = \frac{R^2}{4}, \tag{8.6}$$

which unusually does not depend on θ, telling us that all deflections θ are equally likely. We finally can integrate this up to get the total cross section:

$$\sigma = \int d\Omega D(\theta) = \int_0^\pi d\theta \sin(\theta) \int_0^{2\pi} d\phi D(\theta) = (4\pi)\frac{R^2}{4} = \pi R^2, \tag{8.7}$$

which is the cross-sectional area that the billiard ball presents to the incoming beam of pebbles.

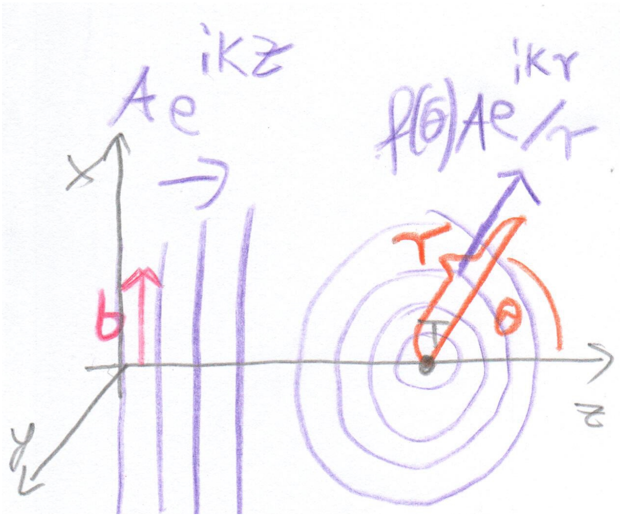
8.2 The quantum scattering problem

In a quantum treatment of scattering, of course we have to replace the fixed positions and momenta of the scatterer (and target) by matter waves. The corresponding wave scattering picture is shown below. To have an as well defined scenario as possible, we give up completely on a fixed position of the projectile prior to collision, but specify its momentum. The projectile is thus coming in as a 3D plane wave $e^{i\mathbf{k}\cdot\mathbf{r}}$, and we will work with a coordinate system where the z-axis is chosen parallel to $\mathbf{k}$ so that this becomes e^{ikz}. The fact that interactions with the target will scatter the projectile into different angles, is then taken into account by allowing for a spherically outgoing radial wave, so that the complete scattering Ansatz becomes

Scattering wavefunction

$$\phi(\mathbf{r}) \approx A\left(e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right). \tag{8.8}$$

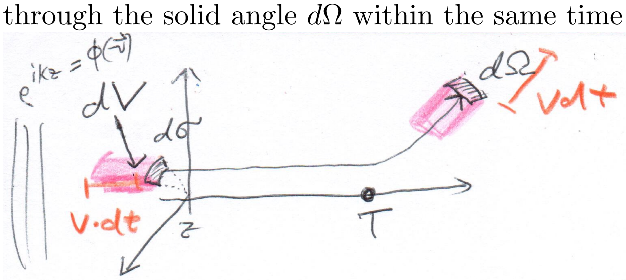
This is sketched in the figure below, which also defines the coordinates.



left: Scattering wavefunction, composed of an incoming plane wave and outgoing spherical wave. We are use a mix of spherical polar coordinates $(r,\ \theta,\ \varphi)$, centered on the target, tand cartesian coordinates (z). Violet lines are equal phase fronts. As usual $k = \sqrt{2mE}/\hbar$.

- The $\approx$ in (8.8) means that the Ansatz is meant only for "large" r, where the projectile has stopped interacting with the target. We call this the "far-field". In other words, if there is a finite range potential $V(r)$, where $r = |\mathbf{x}_{proj} - \mathbf{x}_{targ}|$, we must be outside the range of $V(r)$.
- We are working in the centre-of-mass frame, or perhaps easier to visualize, we assume an infinitely heavy target.
- We assume $V(\mathbf{r})$ is azimuthally symmetric around the z-axis, thus f is not a function of φ. This might not be the case in more complicated scattering problems involving spins and/or external fields, that break spherical symmetry of the scattering potential.
- The factor of $1/r$ in (8.8) already takes into account that the total outgoing probability has to be conserved. To find the outgoing probability we would have to integrate $|\phi(\mathbf{r})|^2$ over a spherical shell, the surface area of which is $4\pi r^2$, hence that factor of r^2 will cancel the one from that denominator. This way we know that at large distances, f should depend on θ only, no longer on r.

Now to connect the scattering wavefunction (8.8) with our earlier definition of the differential cross section (8.3), we want to know the total (infinitesimal) probability dP that a particle in the state $\phi(\mathbf{r})$ moves through the incoming cross section $d\sigma$ in a time interval dt, and then later passes through the solid angle $d\Omega$ within the same time interval.



left: To find dP, we realize that IF the particle is in the volume(s) dV shown in the drawing on the left (compare drawing earlier), it will pass through $d\sigma$ or $d\Omega$ respectively. The probability that it is in that volume is clearly $dP = |\phi(\mathbf{r})|^2 dV$ with $\phi(\mathbf{r})$ from Eq. (8.8).

We can read off

$$dP_{\text{in}} = |\phi(\mathbf{r})|^2 dV = A^2 \underbrace{(d\sigma v dt)}_{=dV},$$

$$dP_{\text{out}} = |\phi(\mathbf{r})|^2 dV = \left|\frac{f(\theta)}{r}\right|^2 \underbrace{(r^2 d\Omega v dt)}_{=dV}. \tag{8.9}$$

These have to be the same along the projectile trajectory $dP_{\text{in}} = dP_{\text{out}}$, due to conservation of probability, hence we deduce the

Differential cross section from scattering wavefunction

$$\frac{d\sigma}{d\Omega} = D(\theta) = |f(\theta)|^2. \tag{8.10}$$

which means that we can extract the differential cross section once we know the scattering wavefunction $\phi(\mathbf{r})$. We can think of (8.8) as the 3D generalisation of the 1D Ansatz (2.28). Same as for that one, this means that we have to determine $f(\theta)$ such that $\phi(\mathbf{r})$ solves the 3D TISE for the scattering problem, with the interaction potential $V(r)$ between projectile and target. Clearly for e.g. scattering of an electron and a proton, we have to solve the same TISE as we solved in week 10 for the Hydrogen atom. However now we are not solving it for bound states, with $E < 0$ but for scattering states, with $E > 0$.

In the following we will see two complementary tricks to solve the 3D TISE for scattering problems, the partial wave expansion and the Born approximation.

8.3 Partial-wave expansion

8.3.1 Expansion in angular momentum or impact parameter

Assuming a spherically symmetric scattering potential $V(\mathbf{r}) = V(r)$, the Hamiltonian commutes with the angular momentum operator, and we know that we can write a solution of the TISE as

$$\phi(\mathbf{r}) = \frac{u_\ell(r)}{r} Y_{\ell m}(\theta, \varphi), \tag{8.11}$$

compare Eq. (4.75). As for Hydrogen, the TISE separates into an angular part (4.42) and a radial part (8.12), where we have already used that the solution of the angular one are spherical harmonics.

Eq. (8.11) represents a fixed angular momentum $\mathbf{L}^2\phi(\mathbf{r}) = \hbar^2\ell(\ell+1)\phi(\mathbf{r})$, and the radial wavefunction fulfills

$$-\frac{\hbar^2}{2m_e}\frac{d^2}{dr^2}u_\ell(r) + \underbrace{\left[V(r) + \frac{\hbar^2}{2m_e}\frac{\ell(\ell+1)}{r^2}\right]}_{\equiv V_{\text{eff}}(r)} u_\ell(r) = E u_\ell(r). \tag{8.12}$$

Here we have $E > 0$ since we are looking for scattering solutions.

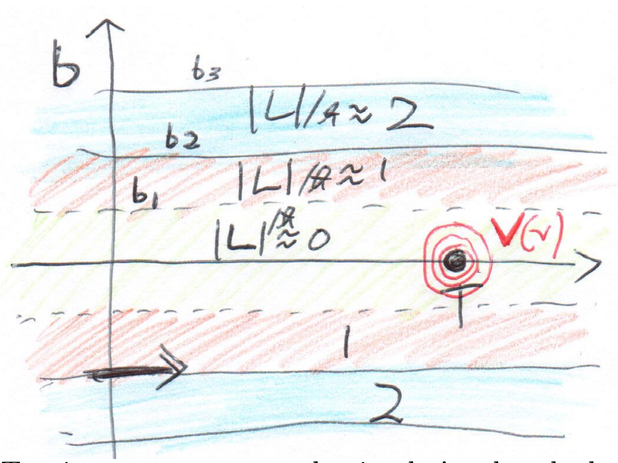
Now we have to build in our scattering boundary conditions, which say that a particle is coming in as a plane wave travelling into the positive z-direction, as expressed in (8.8) and the associated figure. In that equation we could of course write e^{ikz} in spherical polar coordinates, where this becomes $e^{ir\cos\theta}$. This makes it apparent that we ought to be able to expand the θ dependence of that function in terms of spherical harmonics, since these form a basis of all functions defined in terms of two angles θ, φ, see section 4.3. Such an expansion is provided by

Rayleigh's formula: for the expansion of a plane wave in spherical harmonics:

$$e^{ikz} = \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1)j_{\ell}(kr)P_{\ell}(\cos\theta), \tag{8.13}$$

where $j_{\ell}(kr)$ is a spherical Bessel function of the first kind.

Before disecting (8.13) a bit more, let us think about what it would mean to "decompose" the classical incoming state for the scattering problem in terms of (classical) angular momentum. Since $|\mathbf{L}| = pb = \hbar kb$ for impact parameter b, for all $b < b_{\ell} = \ell/k$, we have that $|\mathbf{L}| < \hbar\ell$.

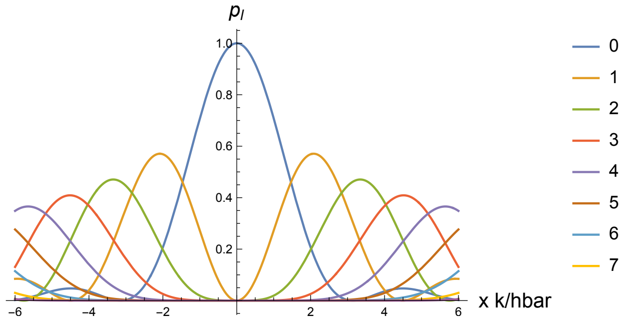


left: Accordingly we can segregate space into cylinders with increasing classical angular momentum with respect to the target, as shown. For a potential $V(r)$ (red) with finite range R_{pot} (say $V(r) \approx 0$ for $r > R_{\text{pot}}$), and small k, we might encounter scenarios where only projectiles with smaller angular momentum "feel' the scattering potential.

Turning to quantum mechanics, let's take a look at what the different contributions ℓ in the formula (8.13) mean. We know that no $m \neq 0$ contributions can arise in (8.11) due to azimuthal symmetry. From (4.48) you can find

$$Y_{\ell}^{0}(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}}P_{\ell}(\cos\theta), \tag{8.14}$$

we can hence write the ℓ'th term in the sum (8.13) as $i^{\ell}\sqrt{(4\pi)}\sqrt{(2\ell+1)}j_{\ell}(kr)Y_{\ell}^{0}$. If there was only a contribution for a single ℓ, then on an x-axis going through the target (that means $x = b$, the impact parameter), the probability density is proportional to $(2\ell+1)|j_{\ell}(kx)|^2$, which we below as a function of $xk/\hbar$.



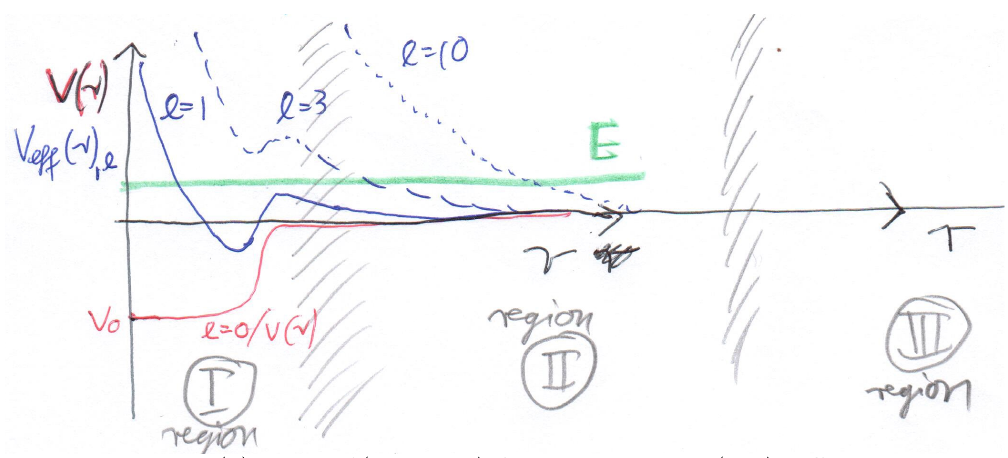
left: Different colors are different ℓ as shown in the legend. You can see that the higher the angular momentum components, the further their radial wavefunction is pushed out, roughly matching the slicing of the impact parameter axis into angular momenta suggested by the above classical picture.

Warning: This picture is intended to give some intuition into decomposing a plane wave in terms of angular momentum. It is a little bit dangerous since we are trying to discuss a fixed position AND fixed angular momentum simultaneously, which we really cannot due to the Heisenberg uncertainty relation.

8.3.2 Interplay with potential range

It is apparent from the diagrams above, that in cases where the range of the potential R_{pot} is less than $1 \times (k)^{-1}$ we would only expect some low angular momentum components to contribute to scattering, since the higher ones "will miss" the potential.

To see how that works out in practice, we have to take a closer look at the radial TISE (8.12)



top: Potential taken as $V(r) \approx -V_0\theta(R_{\text{pot}} - r)$ for this example (red), effective potential V_{eff} for various values of ℓ (blue), some positive scattering energy E (green) and regions I,II,III.

Based on the potentials on the RHS of that, we can consider three regions as sketched above, (I) the scattering region where $V(\mathbf{r})$ must be included, (II) the intermediate region, where we approximate[19] $V(\mathbf{r}) \approx 0$ but consider the centrifugal term $\sim \ell(\ell+1)/r^2$ and (III) the radiation zone, where we neglect both. In the following we look at the structure of solutions for Eq. (8.12) in all these regions, focussing on outgoing waves only (since the incoming part of (8.8) is already sorted out with Eq. (8.13)).

[19]This requires $V(r)$ to drop faster than $1/r^2$, and hence importantly excludes the Coulomb potential

In region (III): Here Eq. (8.12) is simplest

$$\frac{d^2}{dr^2}u_\ell(r) = -k^2 u_\ell(r), \tag{8.15}$$

using $k = \sqrt{2mE}/\hbar$. This has the solution $u(r) = Ce^{ikr} + De^{-ikr}$, which are an outgoing and an incoming spherical wave. For the scattered wave part, we cannot have the latter, hence we set $D = 0$.

In region (II): we see that Eq. (8.12) becomes

$$\frac{d^2}{dr^2}u_\ell(r) - \frac{\ell(\ell+1)}{r^2}u_\ell(r) = -k^2 u_\ell(r), \tag{8.16}$$

which has the general solution $u(r) = Arj_\ell(kr) + Bry_\ell(kr)$, where $j_\ell(kr)$ is a spherical Bessel function of the first kind as used in (8.13) and $y_\ell(kr)$ one of the second kind. We again want to focus solely on the outgoing part contained in $u(r)$, which turns out to be proportional to the linear combination which form a

Spherical Hankel function: of the first kind

$$h_\ell^{(1)}(kr) = j_\ell(kr) + iy_\ell(kr). \tag{8.17}$$

Griffith list a few examples of Hankel functions. Importantly $h_\ell^{(1)}(kr) \to \frac{(-i)^{\ell+1}}{kr}e^{ikr}$ for large kr, which means our solution for region II naturally approaches the r dependence expected in region III.

We now use Eq. (8.13) to expand the incoming wave and Eq. (8.14) (there can be no $m \neq 0$), Eq. (8.11) and our solutions in regions II and II just found, to write the quite generic scattering wavefunction (8.8) in much more detail as the

Partial wave expansion of the scattering wave function (in the outer regions II and III) as

$$\phi(r,\theta,\varphi) = \mathcal{N}\left(\sum_{\ell=0}^{\infty} i^\ell(2\ell+1)\left[j_\ell(kr) + ika_\ell h^{(1)}(kr)\right]P_\ell(\cos\theta)\right), \tag{8.18}$$

where $k = \sqrt{2mE}/\hbar$ depends on the scattering energy, and all information about the scattered wave is contained in the partial wave amplitudes a_ℓ

- Note that it is just a convention to write the coefficient of the outgoing part as $i^{\ell+1}(2\ell+1)ka_\ell$, since we could absorb all the clutter in a_ℓ, which is not specified yet. These coefficients are what became of the constants C in region III and A, B in region II.
- To find the partial wave amplitudes a_ℓ, we have to match (8.17) continuously to the solution of Eq. (8.12) in the inner region I, where the potential is large (this we have not done yet,

since we have not specified $V(r)$). This is similar to our matching solutions in region I, II, III for scattering of the 1D barrier in section 2.2.3 or our matching of WKB solution in various region in section 7.9.

- While we have thus not actually solved the scattering problem, an important achievement is that we now know only the a_ℓ are to be found, and should give us all information on the scattering problem.
- For instance, since at large r we have that $h^{(1)}(kr) \to (-i)^{\ell+1} e^{ikr}/(kr)$, by comparing Eq. (8.23) with Eq. (8.8) we can identify

$$f(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1) a_\ell P_\ell(\cos\theta). \tag{8.19}$$

From this we can find the differential cross section

$$D(\theta) = |f(\theta)|^2 = \sum_{\ell,\ell'=0}^{\infty} (2\ell+1)(2\ell'+1) a_\ell a_{\ell'} P_\ell(\cos\theta) P'_\ell(\cos\theta), \tag{8.20}$$

and the total cross section

$$\sigma = \int d\Omega D(\theta) = 4\pi \sum_{\ell=0}^{\infty} (2\ell+1)|a_\ell|^2. \tag{8.21}$$

To get from (8.20) to (8.21) we used the

Orthogonality of Legendre polynomials:

$$\int d\Omega \sqrt{\frac{2\ell+1}{4\pi}} \sqrt{\frac{2\ell'+1}{4\pi}} P_\ell(\cos\theta) P_{\ell'}(\cos\theta) = \delta_{\ell\ell'} \tag{8.22}$$

- You can see this e.g. from Eq. (4.55), using Eq. (8.14).

How to use Eq. (8.23) is best be seen with an example, that trickily avoids having to solve in a region I, by replacing that with a boundary condition:

Example 64, Quantum scattering off a hard sphere: We are now in a position to revisit example 63, but this time quantum mechanical. Hard sphere here means that $V(\mathbf{r}) = \infty$ if $|\mathbf{r}| < R$ and $V(\mathbf{r}) = 0$ otherwise. As usual with infinite potential walls, we thus have the boundary condition $\phi(R, \theta, \varphi) = 0$ for all angles. Using (8.23) this implies

$$0 = \mathcal{N} \left(\sum_{\ell=0}^{\infty} i^\ell (2\ell+1) \underbrace{\left[j_\ell(kR) + ika_\ell h^{(1)}(kR) \right]}_{\stackrel{!}{=}0} P_\ell(\cos\theta) \right), \tag{8.23}$$

where the conclusion under the braces follows because the Legendre polynomials $P_\ell(\cos\theta)$ are linearly independent.

Example continued: We can thus extract all

$$a_\ell = i\frac{j_\ell(kR)}{kh^{(1)}(kR)}, \tag{8.24}$$

which means we have now completely solved the quantum scattering problem for the hard sphere.
We can now insert the a_ℓ into (8.21) and in the limit $kR \gg 1$ (see Griffith) find a total cross section

$$\sigma = 4\pi R^2, \tag{8.25}$$

four times what we found classically (Eq. (8.7)). This corresponds to the surface area instead of the geometrical cross section of the sphere.

As suggested earlier, for short range potential we might get away with only few contributing partial waves:

Example 65, S-wave scattering of ultracold atoms: Let's assume a very short range potential between atoms and very slow atoms, such that $kR_{\text{pot}} \ll 1$. Alternatively think of $E \approx 0$. We can then read off the drawing[a] at the beginning of section 8.3.2, that except for $\ell = 0$, none of the radial wavefunctions $u_\ell(r)$ for partial waves should reach $\mathbf{r}) = 0$ and thus feel the potential. We thus conclude that for very low energy scattering from short ranged potential, only the $\ell = 0$ portion of the partial wave expansion is important. This is called s-wave scattering.
The argument could be made more mathematical by going through Eq. (8.16) andEq. (8.15) again, neglecting k in the right places and connecting solutions in region II and II (see Landau and Lifshitz, Quantum mechanics, ¶132). You can then show that the contribution of the ℓ'th partial wave to the total cross section scales like $k^{2\ell}$, thus for small k only the lowest is relevant.
Once we know only $\ell = 0$ as important, and recall that $Y_0^0 = 1/\sqrt{4\pi}$ (just a constant), we see that we can write (8.8) as

$$\phi(\mathbf{r}) \approx A\left(e^{ikz} + f\frac{e^{ikr}}{r}\right), \tag{8.26}$$

i.e. f is just one number. This is usually expressed as $f = -a_s$, where a_s is called the (s-wave) scattering length. To find it, we still would have to solve the TISE in region I, or measure it in an experiment.

[a] As for any TISE, the solution will drop exponentially once $E < V(x)$.