14 Using Partial Waves

14.1 Impact Parameter and Classical Analogies

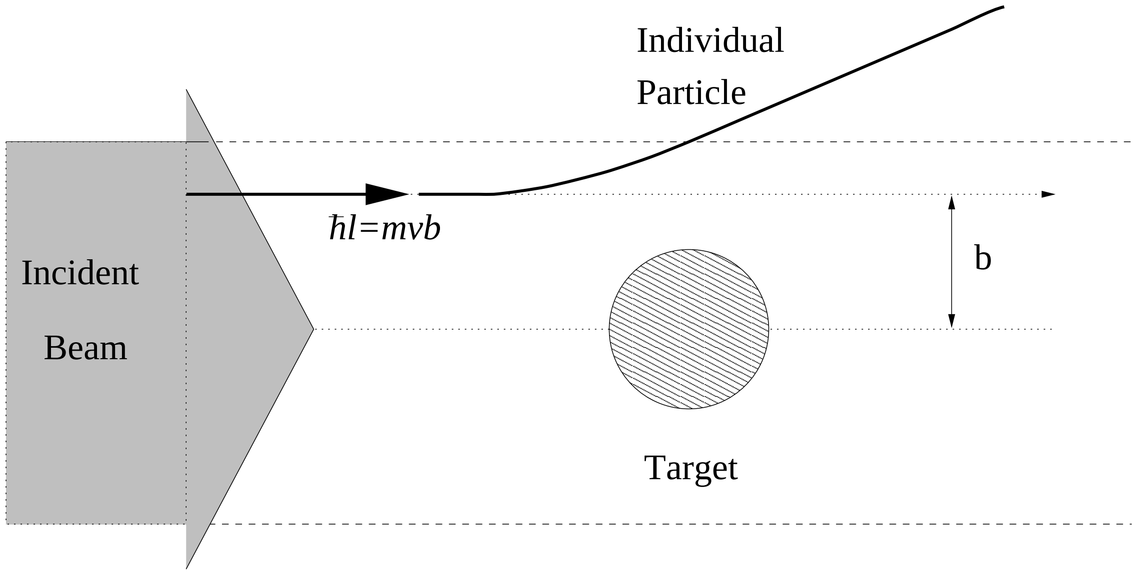

Figure 14: Relation between classical and quantum angular momentum

Knowing the impact parameter gives us some classical idea of whether a scattering event is likely. If the impact parameter is larger than the range of the potential, then classically the particles would miss. In the quantum case, we expect this to mean that the phase shift for that angular momentum is zero, and hence that the contribution from that term in the expansion is zero. Thus at a given incoming momentum, $\hbar k$, we can determine how many terms in the partial wave expansion to consider from $\hbar k b_{max} \approx l_{max}\hbar$, where b_{max} is the maximum impact parameter for classical collision, i.e. the range of the potential.

14.2 S-wave scattering

Although exact at all energies, the partial wave method is most useful for dealing with scattering of low energy particles. This is because for slow moving particles to have large angular momentum ($\hbar kb$) they must have large impact parameters b. Classically, particles with impact parameter larger than the range of the potential miss the potential. Thus for scattering of slow-moving particles we need only consider a few partial waves, all the others are unaffected by the potential ($\delta_l \approx 0$). Thus partial waves and the Born approximation are complementary methods, good for slow and fast particles respectively.

For very low energy we need consider only the first term in the partial wave expansion. This is known as *S-wave scattering*. In this case it is possible to solve for the differential cross section, since only the first term in the series for $f(\theta)$ is involved: Since the angular variation is $P_0(\cos\theta) = 1$ the scattering is isotropic.

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = k^{-2}\sin^2\delta_0$$

At higher energies, other angular momentum components come into play. For a given l component, scattering is maximised for $\delta_l = \pi/2$.

14.3 Resonance

In some cases where a potential has a bound state of particular angular momentum, the scattering of particle with that angular momentum will be especially enhanced. In such cases the total scattering cross section will show a peak, and the angular distribution will be characteristic of the appropriate $P_l(\cos\theta)$. This very strong scattering is known as resonance and is a powerful method for studying bound states.

14.4 Example of S-wave scattering - Attractive square well potential

An example where we can solve for the phase shift is the 3D-square well potential:

$(V(r < R) = -V_0;\ V(r > R) = 0)$.

For the $l = 0$ case the radial equation with $U_0 = R_0 r$ is

$$\frac{d^2u_0(r)}{dr^2} + \frac{2\mu}{\hbar^2}[E - V(r)]u_0(r) = 0$$

The solutions to this are familiar from the 1D square well. If we write

$$K_0 = \sqrt{2\mu[E + V_0]}/\hbar; \qquad\qquad K = \sqrt{2\mu E}/\hbar$$

then for $r < R$, $u(r) = A\sin K_0 r + B\cos K_0 r$.

and for $r > R$, $u(r) = C\sin Kr + D\cos Kr$. which can easily be written in a different form to show the appropriate phase shift δ_0: $u(r) = F\sin(Kr + \delta_0)$ where $(C = F\cos\delta_0\ ;\ D = F\sin\delta_0)$

As with the 1D square well, the boundary conditions are that u and $\frac{du}{dr}$ are continuous at R, which lead to:

$$K\tan K_0 R = K_0\tan(KR + \delta_0) \quad \text{or} \quad \delta_0 = \tan^{-1}\left(\frac{K}{K_0}\tan K_0 R\right) - KR$$

In the low energy case $KR \ll 1$, we obtain maximum scattering ($\sin^2\delta_0 \to 1$) when $K_0 R = (n + \frac{1}{2})\pi$, when the scattering cross section is $\sigma = 4\pi/K^2$. This is an example of *s-wave resonance.*

In the same slow particle limit $K \ll K_0$, and assuming that $\tan K_0 R$ is not very large: $\delta_0 \approx \sin\delta_0$.

$$\sigma \approx 4\pi R^2\left(\frac{\tan K_0 R}{K_0 R} - 1\right)^2$$

This correctly predicts that when $\tan K_0 R = K_0 R$ the scattering cross section will be zero.

There are a few features of the square-well which also apply in more general cases. Assuming K_0 is basically a measure of the potential depth.

- For weak coupling $K_0 R \ll 1$, $\delta_0(K) \to 0$ as $K \to 0$
- When $K_0 R$ approaches $\pi/2$ the potential is almost able to bind an s-wave bound state. Now the phase shift $\delta_0(K) \to \pi/2$ and the cross section *diverges* like K^{-2} as $K \to 0$. This is known as zero energy resonance.
- If E is high enough that $\delta_l = (n + \frac{1}{2})\pi$ for $l \neq 0$ the scattering cross section can become especially high due to another angular momentum component - p-wave resonance for $l = 1$, d-wave resonance for $l = 2$ etc. In these cases the eigenfunction becomes large near to the potential. The potential is said to have *virtual states* at the resonance energies.

- *Levinson's Theorem* states that $$\lim_{k \to 0} \delta_l(k) = n_l \pi$$ where n_l is the number of bound states with angular momentum l.

- Whenever $\delta_0(K) = n\pi$, for s-wave scattering, $\sigma = 0$. Thus for certain energies of the incoming particle, the scattering is extremely small. This condition can only be consistent with the condition for s-wave scattering ($KR \ll 1$) if the potential is attractive ($V_0 < 0$).

- $\delta_0(K)$ tends to decrease with increasing K. This can be understood physically as the faster particles having less time to interact and thus experiencing smaller phase shifts. As $K \to \infty$, $\delta_l(K) \to 0$ because the potential is now weak relative to the particle energy. Of course $\sigma(K \to \infty)$ decreases even more quickly because of the K^{-2} term.

14.5 Partial Waves in the Classical Limit - Hard Spheres

Consider the scattering of a small hard sphere (radius x_m, mass m) by a large hard sphere (X_M, M). Firstly we transform the problem to the centre of mass reference frame where it becomes that of a single effective particle of mass $\mu = mM/(m+M)$ moving in a hard sphere potential ($V(r < r_H = X_M + x_m) = \infty$). Thus the boundary condition is $R_l(r_H) = 0$.

Consider the classical limit, where the sphere radius is much larger than the de Broglie wavelength, $kr_H \gg 1$. Up to $l = Kr_H$ the phase shift is enormous and $\sin\delta_l$ could have any value. For $l > Kr_H$ the impact parameter is so large that the particles miss and $\delta_l = 0$. Thus we can write the scattering cross section:

$$\sigma = \frac{4\pi}{K^2} \sum_{l=0}^{l=Kr_H} (2l+1)\frac{1}{2}$$

where we replace $\sin^2\delta_l$ with its average value of $\frac{1}{2}$.

Since Kr_H is large, we can replace the sum by an integral and take only the leading term; $(Kr_H)^2 \gg Kr_H$:

$$\sigma \approx \frac{2\pi}{K^2} \int_{l=0}^{l=Kr_H} (2l+1)dl \approx 2\pi {r_H}^2$$

This result should send us rushing back to look for the extra factor of 2, since the cross-section of a sphere might be expected to be $\pi {r_H}^2$. In fact, though, the analysis is correct and closer analysis of the θ dependence of the wavefunction shows that half the amplitude is diffracted into the classical 'shadow' of the sphere to cancel the amplitude of the unscattered wave there.

14.6 Ramsauer-Townsend effect

This is the name given to the fact that electrons with energy about 1eV can pass almost freely through Xe, Kr, and Ar:- there is a sharp minimum in electron scattering cross-section for these noble gases.

Due to polarisation of these atoms by the incoming electron the potential appears to increase as K increases (more localised electrons are better able to polarise the atom). Thus $\delta_0(k \to 0) = n\pi$, in accordance with Levinson's theorem, and δ_0 initially increases as k increases, before eventually decreasing. Thus at a certain value of k, the phase shift is again $\delta_0(k) = n\pi$, and the total scattering cross section σ_T has an abrupt minimum. Although there are subsequent s-wave minima at e.g. $\delta_0(k) = (n-1)\pi$, these occur at sufficiently large values of k that s-wave scattering is no longer dominant.

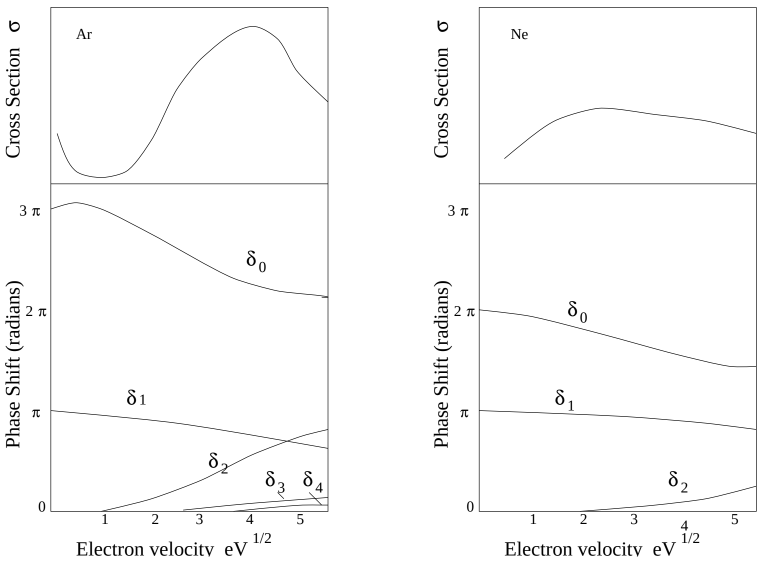

Figure 15: Minimum in scattering cross section in Ar due to $\delta_0 = 3\pi$; No such effect in Ne due to weaker polarisation.

By contrast, neon and helium have lower polarisability, due to fewer bound electrons. Thus the phase shift δ_0 decreases monotonically with k from $n\pi$ at $k = 0$ at there is no low-energy minimum.

Higher l phase shifts may increase with k because higher k implies smaller impact parameter (classically, more chance of hitting the atom). The cross section increases more slowly due to the additional K^{-2} dependence. The maximum in the Ar cross section at about 13eV is mainly due to the d-wave $\delta_2 = \pi/2$.

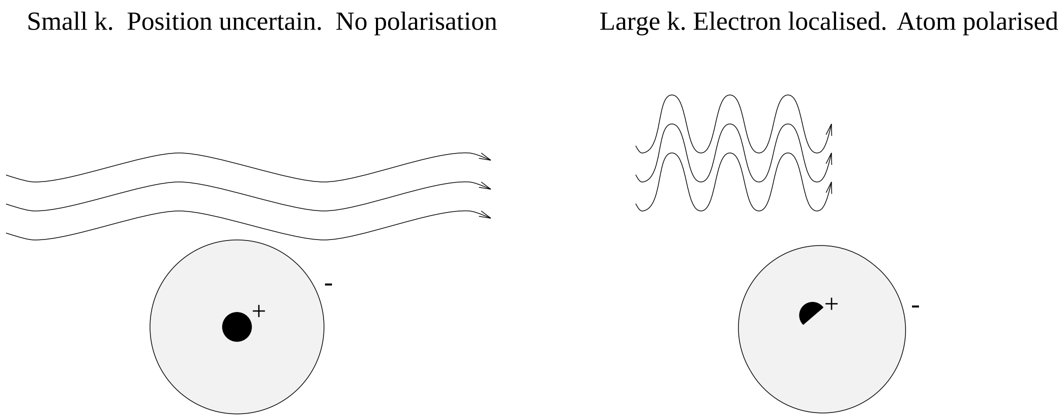

Figure 16: More-localised electrons polarise atoms and thus increase the attractive potential