16.1 Using conservation of angular momentum

One method of solving the scattering problem is to use the Born Approximation. This is a perturbation method based on the Fermi Golden Rule and is therefore valid for short-ranged, weak potentials. For the case of a central potential a more general method exists: Partial waves.

It is well known that a particle moving in a central potential experiences no torque (about the potential origin), and therefore conserves angular momentum. In the quantum case angular momentum is quantised, so the scattering does not change the angular momentum quantum number l. Partial waves proceeds by a 'divide and conquer' strategy of expanding the incident and scattered fluxes in a basis set of distinct angular momentum. The angular parts of this basis are unaffected by the scattering, thus we need consider only the 1D radial problem. Moreover, for a conservative potential, the energy of the particles is unaffected, thus $|k| = |k'|$, so all that a central potential can achieve is a change of *phase*.

Like the Born approximation, the derivation of the Partial Wave equation is complicated, but it can be done for a general potential, so once we have the result we can just use it.

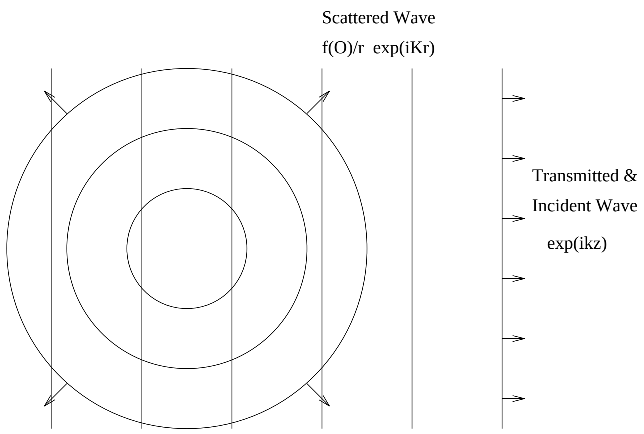

Figure 15: Plane wave in, radial wave out. $|\Psi\rangle = e^{ikz} + f(\theta)e^{ikr}/r$

16.2 Digression: Expanding a plane wave in an angular momentum basis set

A preliminary step in partial wave analysis is to expand the incident plane wave in a set of partial waves. The solution to the Schroedinger equation for a free particle in spherical polars can be separated into three parts:

$$\text{Incident free particle wavefunction} = e^{iKz} = e^{iKr\cos\theta} = R(r)\Theta(\theta)\Phi(\phi)$$

Solving for Φ is trivial - there is no ϕ dependence of $e^{iKr\cos\theta}$ - so $\Phi(\phi) = 1$. Θ is also straightforward, since we have already solved the Schroedinger equation for hydrogen, and the potential has the same θ dependence (i.e. none), so the Θ functions must be the Legendre polynomials $P_l(\cos\theta)$ which are orthogonal and normalised to $\langle P_l P_k\rangle = \frac{2}{2l+1}\delta_{kl}$. By analogy with hydrogen (though with V=0), R(r) must now be a solution to the equation:

$$\frac{1}{r^2}\frac{d}{dr}(r^2\frac{dR}{dr}) - \frac{l(l+1)}{r^2}R + \frac{2\mu}{\hbar^2}ER = 0$$

Because we are describing free particles, $E > 0$ and E is not quantised. Incoming beams of any energy can be treated. The solutions to this equation are well known to mathematicians, and can be found in most quantum mechanics books. They are the Spherical Bessel Functions: $j_l(Kr)$.

Thus we can expand $e^{iKr\cos\theta}$ in spherical harmonics and spherical Bessel functions - a complete set of orthonormal basis states which are eigenstates of the angular momentum: $\hat{L}^2|j_l(Kr)P_l(\cos\theta)\rangle = l(l+1)\hbar|j_l(Kr)P_l(\cos\theta)\rangle$. Of the complete set of spherical harmonics, we need only the Legendre polynomials $P_l(\cos\theta) = Y_{l0}$ because of the cylindrical symmetry ($\Phi(\phi) = 1$). We can write the plane wave along z in this basis set, with coefficients a_n

$$\exp(iKr\cos\theta) = \sum_{n=0}^{\infty} a_n j_n(Kr) P_n(\cos\theta)$$

whence, multiplying by $P_l(\cos\theta)$ and integrating over θ to pick out a specific component:

$$\langle P_l|\exp(iKr\cos\theta)\rangle = \sum_{n=0}^{\infty} a_n j_n(Kr)\langle P_l|P_n\rangle = \frac{2}{2l+1}a_l j_l$$

Integrating the left hand side by parts gives a term proportional to r^{-1} and a series of terms of higher order r^{-n}. Taking the limit as $r \to \infty$, where only the r^{-1} term is significant:

$$\frac{2}{2l+1}a_l j_l = \frac{1}{iKr}[P_l(\cos\theta)\exp(iKr\cos\theta)]_{\cos\theta=-1}^{\cos\theta=1} \qquad r \to \infty$$

This boundary condition is sufficient to determine the a_l.

Now, for Legendre polynomials $P_l(\cos\theta = 1) = 1$ and $P_l(\cos\theta = -1) = (-1)^l = e^{il\pi}$ so that:

$$\frac{2}{2l+1}a_l j_l = \frac{1}{iKr}[e^{iKr} - e^{il\pi - iKr}] \qquad r \to \infty$$

which after a bit of manipulation (use $e^{il\pi/2} = i^l$) becomes:

$$a_l j_l(Kr) = (2l+1)i^l \frac{\sin(Kr - l\pi/2)}{Kr} \qquad r \to \infty$$

For the Kr dependence to be correct, we must have:

$$j_l(Kr) = \frac{\sin(Kr - l\pi/2)}{Kr} \qquad r \to \infty$$

which can be confirmed by comparing the form of the Bessel function at $r \to \infty$ with the plane wave. Thus $a_l = (2l+1)i^l$.

Finally, we can write:

$$\exp(iKr\cos\theta) = \sum_{l=0}^{\infty} i^l j_l(Kr)(2l+1)P_l(\cos\theta)$$

which is the representation of a plane wave as a linear combination of partial waves with distinct angular momentum. This is the starting point for partial wave analysis. Because it is independent of the scattering potential we do not need to repeat this expansion (or one like it) every time we do a partial wave calculation: we just use the result.

Note the term (2l+1). This can be related to the classical 'impact parameter' mentioned above. The angular momentum of a particle of velocity v is $mvb = \sqrt{l(l+1)}\hbar$. Thus a classical (large l) particle with angular momentum $l\hbar$ would pass between a ring of radius $b = l\hbar/mv$ and one of radius $b = (l+1)\hbar/mv$. The area between these rings is $(2l+1)\pi(\hbar/mv)^2$ so for a uniform beam the probability of a particle having angular momentum l is proportional to (2l+1).

16.3 Incident and Scattered Flux

If can write the solution to the Schroedinger equation $|\Psi\rangle$ at large r in the form of an incident plane wave and a scattered radial wave:

$$|\Psi\rangle = \text{IncidentWave} \ + \ \text{ScatteredWave} \ = \ \exp iKz + \frac{f(\theta)}{r}\exp iKr$$

Then the incident flux is the product of the probability density and the particle velocity $I = ve^{iKz}e^{-iKz} = v = \hbar k/m$. Likewise the scattered flux must have a radial function which gives a normalisable plane wave (e^{-iKr}/r), and a θ dependence arising from the scattering, which we call $f(\theta)$. By symmetry, there is no ϕ dependence. Thus the scattered flux per unit area will be: $vf^*(\theta)f(\theta)/r^2$.

Thus $d\sigma/d\Omega = S(\theta)/I = f^*(\theta)f(\theta)$, and all we need do is calculate $f(\theta)$.

16.4 Solving the Schoedinger Equation - the Phase Shifts

In the previous section we solved this problem without the potential (i.e. $f(\theta) = 0$), we now solve it with the central potential. For a spherically symmetric potential, the angular part of the Hamiltonian is the same as the previous section, because the potential is independent of ϕ and θ, so the analysis is the same except the equation for $R(Kr)$, which becomes:

$$\frac{d^2u_l(r)}{dr^2} - \frac{l(l+1)}{r^2}u_l(r) + \frac{2\mu}{\hbar^2}[E - V(r)]u_l(r) = 0$$

where we set $u_l(r) = rR_l(r)$, the same substitution as in the atomic hydrogen problem.

If we look at the limit of large $R(Kr \to \infty)$, where the detector in any experiment would be stationed, we find $V(r \to \infty) = 0$ and so $R_l(Kr \to \infty)$ describes a free particle. The solution must therefore tend to the same limit as $j_l(Kr \to \infty)$, though perhaps with different phase:

$$R_l(Kr) = \sin(Kr - l\pi/2 + \delta_l)/Kr$$

This is always a solution at $r \to \infty$ provided that $V(r) \to 0$ faster than $1/r$ (Localised potential).

Thus to perform partial wave analysis we need to solve the radial Schroedinger equation for $R_l(Kr)$ for each angular momentum component.

The wavefunction at long range describes a free particle with the same —K— as the incident beam. The only possible effect of the conservative, central potential is to change the *phase* of plane wave by δ_l. The limit of $r \to \infty$ for each solution can be expressed by a single number: the phase shift δ_l.

16.5 Obtaining Cross sections

Recalling that to get cross sections we need to find $f(\theta)$, we express Ψ in the appropriate form at $R \to \infty$.

$$\Psi = e^{iKz} + f(\theta)\frac{e^{iKr}}{r} = \sum_{l=0}^{\infty} i^l j_l(Kr)(2l+1)P_l(\cos\theta) + f(\theta)\frac{e^{iKr}}{r} = \sum_{l=0}^{\infty} b_l R_l(Kr)P_l(\cos\theta)$$

where b_l are expansion coefficients for the expression of Ψ in the partial wave basis, the equivalent of the a_l for the expression of a free particle in the partial wave basis.

We already know the $r \to \infty$ values for j_l and R_l. Using the limiting values of $j_l(Kr \to \infty)$, writing the equation above in terms of complex exponentials and multiplying by $2iKr$ we find:

$$\sum_{l=0}^{\infty} i^l [e^{i(Kr - l\pi/2)} - e^{-i(Kr - l\pi/2)}](2l+1)P_l(\cos\theta) + 2iKf(\theta)e^{iKr} = \sum_{l=0}^{\infty} b_l [e^{i(Kr - l\pi/2 + \delta_l)} - e^{-i(Kr - l\pi/2 + \delta_l)}]P_l(\cos\theta)$$

Comparing the coefficients of the e^{-iKr} term, we can solve for the expansion coefficients b_l

$$(2l+1)i^l e^{il\pi/2} = b_l e^{il\pi/2 - i\delta_l} \quad ; \quad b_l = (2l+1)i^l e^{i\delta_l}$$

and now, using these values for b_l we can compare the coefficients of the e^{iKr} terms, and after a little manipulation of complex exponentials, we find:

$$f(\theta) = K^{-1} \sum_{l=0}^{\infty} (2l+1)e^{i\delta_l} \sin\delta_l P_l(\cos\theta)$$

From this we can calculate $d\sigma/d\Omega = |f(\theta)|^2$ and $\sigma = 2\pi \int |f(\theta)|^2 d\theta$. Note that $d\sigma/d\Omega$ involves the product of two series, and thus contains many cross terms. In general it is very complicated.

However, when integrated over all θ these cross terms vanish due to orthogonality of the Legendre polynomials $\langle P_l | P_{l'} \rangle = 0$ $(l \neq l')$. Thus the total cross section, expressed in partial waves, has a particularly simple form:

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

Hence the scattering cross sections are completely determined by $|K|$ and the phase shifts δ_l. For a given problem, all we must calculate are the δ_l, then we can simply apply the result above for σ.

Thus all the effect of the potential on a given partial wave in contained in a single number - the phase shift. This is the amount by which can be imagined as the amount a given partial wave is pulled in by the potential. The phase shifts must be obtained by solving the radial equation for $R_l(Kr)$ and comparing with $j_l(Kr)$ at large r for each l. Although the analysis done so far is valid for all problems, for a specific problem, one must still evaluate the phase shifts and solve the radial equation.

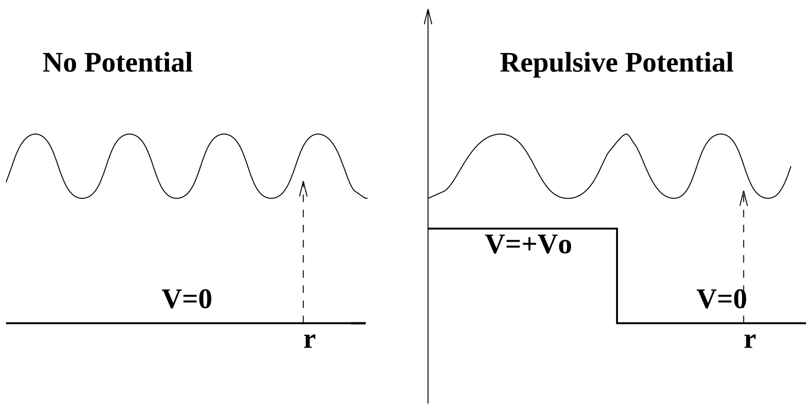

Figure 16: Radial wavefunctions, $u_l(r) = rR(r)$ showing phase difference at r due to short-ranged potential. The attractive potential pulls in the wave giving negative δ_l, while the repulsive potential pushes out the wave for positive δ_l

17 Using Partial Waves

17.1 Impact Parameter and Classical Analogies

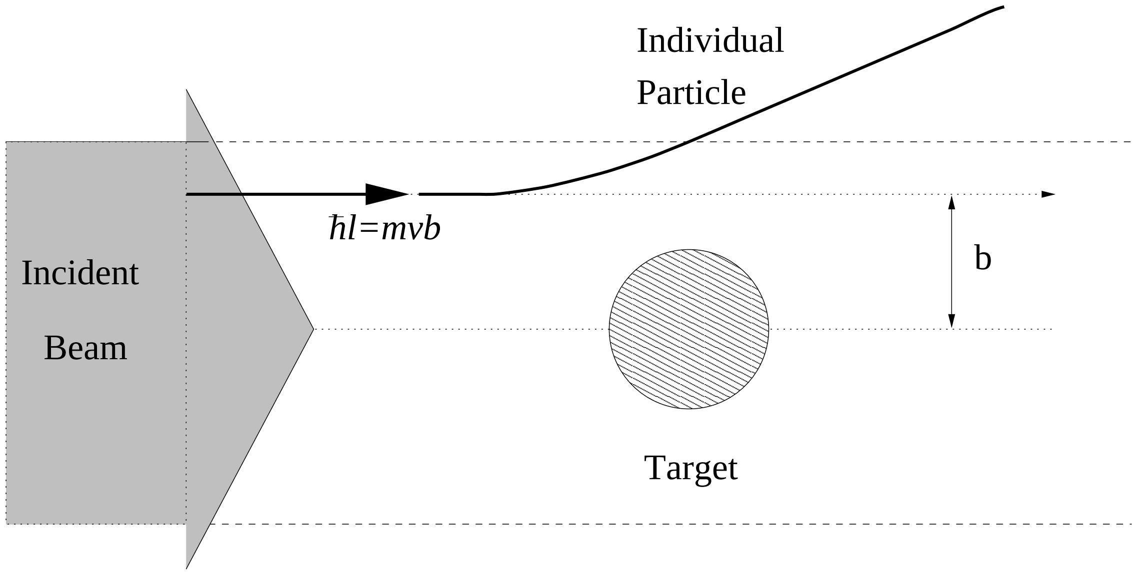

Figure 17: Relation between classical and quantum angular momentum

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.

17.2 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.

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

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

17.3 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.

17.4 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

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

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:

$$K\tan K_0R = K_0\tan(KR + \delta_0) \quad \text{or} \quad \delta_0 = \tan^{-1}\left(\frac{K}{K_0}\tan K_0R\right) - KR$$

In the low energy case $KR \ll 1$, we obtain maximum scattering ($\sin^2\delta_0 \to 1$) when $K_0R = (n+\frac{1}{2})\pi$, 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 $\tan K_0R$ is not very large: $\delta_0 \approx \sin\delta_0$.

$$\sigma \approx 4\pi R^2\left(\frac{\tan K_0R}{K_0R} - 1\right)^2$$

This correctly predicts that when $\tan K_0R = K_0R$ 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 $K_0R \ll 1$, $\delta_0(K) \to 0$ as $K \to 0$
- When K_0R 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.

17.5 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.

17.6 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.

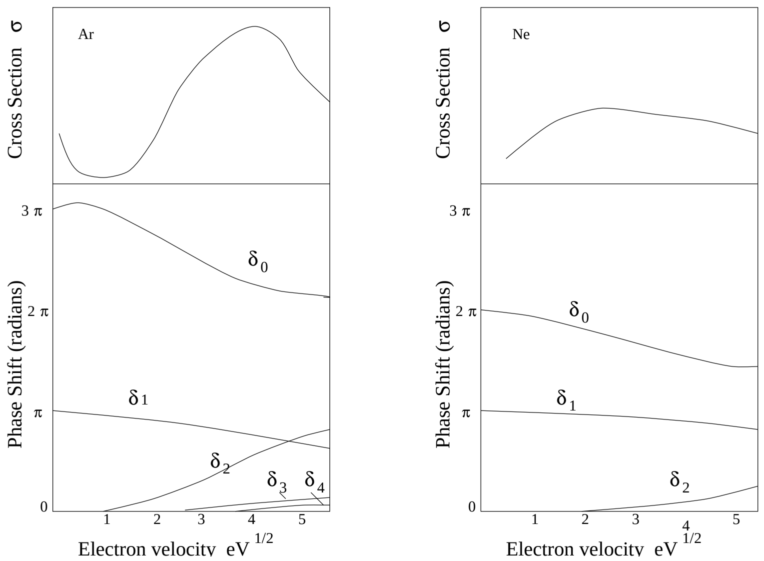

Figure 18: Minimum in scattering cross section in Ar due to $\delta_0 = 3\pi$; No such effect in Ne due to weaker polarisation.

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 $\delta_2 = \pi/2$.

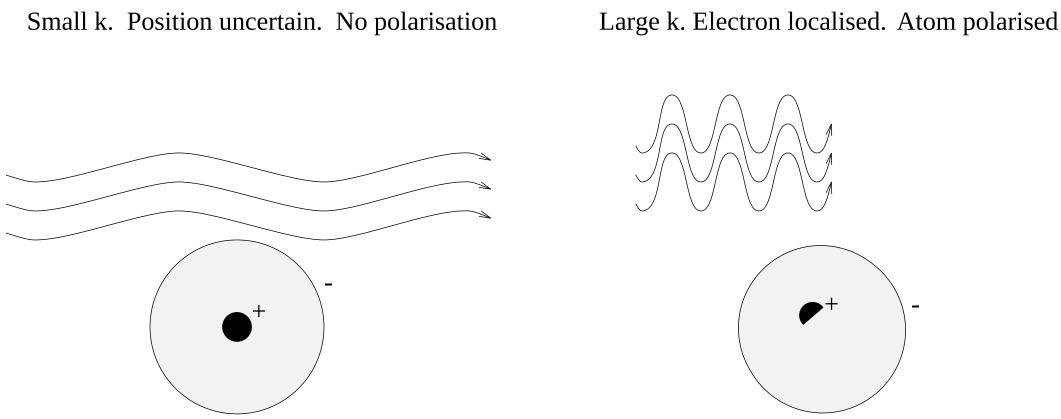

Figure 19: More localised electrons polarise atoms and thus increase the attractive potential