

Chapter 2

Scattering Theory

2.1 Definition of the scattering problem

Physical importance of scattering experiments:

Probing the interactions of the scattered particles with the scattering center, i.e. the microscopic properties (scattering potential) of the scatterer.

We will consider only potential scattering in the non-relativistic case, i.e. the spin is conserved, and particle-antiparticle pair creation does not occur.

Scattering experiment and definition of parameters

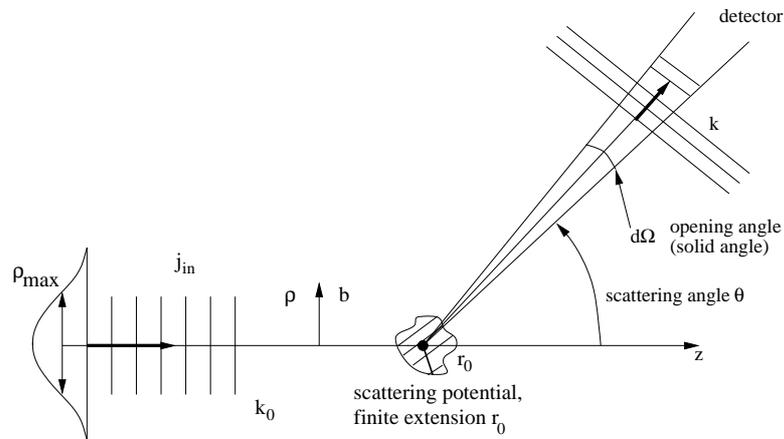


Figure 2.1: Scattering problem

- incident *plane* wave: $\vec{k}_0 \parallel \hat{z}$ for distance from scatterer $r \gg r_0$,
finite extension ρ_{\max} in direction perpendicular to \vec{k}_0 ; $r \gg \rho_{\max} \gg r_0$
- outgoing plane wave: \vec{k} for distance from scatterer $r \gg r_0$
- impact parameter b : distance from scattering center in direction perpendicular to \vec{k}_0

Physically, one is interested in the fraction of the incoming particles that are scattered into a solid angle Ω centered around a scattering angle (θ, ϕ) .

Definition: Differential scattering cross section

$$\frac{d\sigma(\theta, \phi)}{d\Omega} d\Omega := \frac{\frac{\text{number of particles scattered into } d\Omega}{\text{time interval } \Delta t}}{\frac{\text{number of incident particles}}{\text{times interval } \Delta t \cdot \text{cross sectional area } \Delta A}} \quad (2.1)$$

Calculation of $d\sigma/d\Omega$:

1. The scattering problem is the solution of the stationary Schrödinger equation (stationary incoming current) with special boundary conditions. For a sufficient strongly localized scattering potential (e.g. $V(\vec{r}) \sim e^{-r/r_0}$) the ingoing and the outgoing waves are solutions of the Schrödinger equation.

Total solution of $H = H_{\text{kin}} + V$:

$$\psi_k = \psi_{\text{in}} + \psi_{\text{sc}} \quad (2.2)$$

with

- $\psi_{\text{in}}(\vec{r}) = e^{i\vec{k}_0\vec{r}} e^{-iEt}$, $E = \frac{\hbar k_0^2}{2m}$
centered perpendicular to \vec{k}_0 around mean impact parameter $\langle b \rangle$.
- $\psi_{\text{sc}}(\vec{r})$ has only outgoing components, and is for $r \gg r_0$ solution of the free Schrödinger equation.

$\vec{k}_0 \parallel \hat{z}$, $k_0 \equiv k$:

$$\psi_k = e^{ikz} + \psi_{\text{sc}}(r, \theta, \phi) \quad (2.3)$$

$$-\frac{\hbar^2}{2m} \vec{\nabla}^2 \psi_{\text{sc}}(\vec{r}) = E \psi_{\text{sc}}(\vec{r}), \quad r \rightarrow \infty \quad (2.4)$$

Using $E = \frac{\hbar^2 k_0^2}{2m}$ one obtains:

$$(\vec{\nabla}^2 + k_0^2)\psi_{\text{sc}} = 0 \quad (2.5)$$

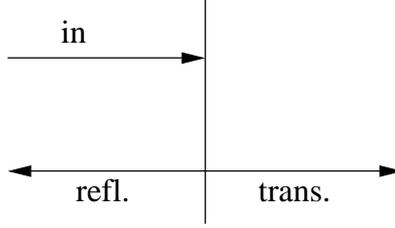


Figure 2.2: Analogous to 1 dimension

Since we are interested in the angle dependence of ψ_{sc} for $r \rightarrow \infty$, and since equation (2.5) is radially symmetric around the scattering center $\vec{r} = 0$, it is useful to expand ψ_{sc} in terms of spherical harmonics $Y_l^m(\theta, \phi)$.

$$\psi_{\text{sc}}(r \rightarrow \infty, \theta, \phi) = \sum_{l,m} [A_l j_l(k_0 r) + B_l n_l(k_0 r)] Y_l^m(\theta, \phi) \quad (2.6)$$

where $j_l(k_0 r)$ (Bessel functions) and $n_l(k_0 r)$ (von Neumann functions) are the solutions of the free radial Schrödinger equation.

$$\left(-\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) \begin{pmatrix} j_l(k_0 r) \\ n_l(k_0 r) \end{pmatrix} = k_0^2 \begin{pmatrix} j_l(k_0 r) \\ n_l(k_0 r) \end{pmatrix} \quad (2.7)$$

where

$$k_0^2 = \frac{2mE}{\hbar^2}. \quad (2.8)$$

The asymptotic behavior of the Bessel and von Neumann functions read:

$$j_l(k_0 r) \xrightarrow{r \rightarrow \infty} \sin\left(k_0 r - l\frac{\pi}{2}\right) \frac{1}{k_0 r} \quad (2.9)$$

$$n_l(k_0 r) \xrightarrow{r \rightarrow \infty} \cos\left(k_0 r - l\frac{\pi}{2}\right) \frac{1}{k_0 r} \quad (2.10)$$

both nonsingular for $r \rightarrow \infty$.

ψ_{sc} consists of only outgoing waves:

$$A_l j_l(k_0 r) + B_l n_l(k_0 r) \sim e^{ik_0 r} \quad (r \rightarrow \infty) \quad (2.11)$$

With the asymptotic forms of $j_l(k_0r)$ and $n_l(k_0r)$ one finds:

$$\frac{1}{2} \left[\left(A_l + \frac{1}{i} B_l \right) e^{i(k_0r - l\frac{\pi}{2})} + \underbrace{\left(A_l - \frac{1}{i} B_l \right) e^{-i(k_0r - l\frac{\pi}{2})}}_{=0} \right] \frac{1}{k_0r} \quad (2.12)$$

$$\Rightarrow \quad \boxed{A_l = -iB_l} \quad \boxed{e^{-il\frac{\pi}{2}} = (-i)^l} \quad (2.13)$$

$$\psi_{\text{sc}}(\vec{r}) \xrightarrow{r \rightarrow \infty} \frac{e^{ik_0r}}{k_0r} \sum_{l,m} (-i)^{l+1} B_l Y_l^m(\theta, \phi) \quad (2.14)$$

$$= =: \frac{e^{ik_0r}}{r} f(\theta, \phi) \quad (2.15)$$

$$\psi_{\vec{k}} \xrightarrow{r \rightarrow \infty} e^{ikz} + f(\theta, \phi) \frac{e^{ik_0r}}{r} \quad (2.16)$$

$f(\theta, \phi)$ is called *scattering amplitude*:
 $f(\theta, \phi) = \frac{1}{k_0} \sum_{l,m} (-i)^{l+1} B_l Y_l^m(\theta, \phi)$

(2.17)

The coefficients B_l are to be determined such that $\psi_{\vec{k}}$ is a solution of the Schrödinger Gleichung in the region of the scattering potential (= matching boundary conditions for a given potential).

Note:

The r-dependence in (2.16) is expected, since it leads to a radial component of the current density

$$j_r = \frac{\hbar}{2mi} \left[\psi_{\text{sc}}^* \left(\frac{\partial}{\partial r} \psi_{\text{sc}} \right) - \left(\frac{\partial}{\partial r} \psi_{\text{sc}}^* \right) \psi_{\text{sc}} \right] \sim \frac{1}{r^2} \quad (2.18)$$

i.e. to an overall current conservation

$$\int_{r_0} dS_{r_0} j_{r_0} = I = \int d\Omega r_0^2 j_{r_0} = \text{const.}(r_0). \quad (2.19)$$

2. Computing $d\sigma/d\Omega$ from $f(\theta, \phi)$:

Incoming and scattered current density:

$$\vec{j}_{\text{in}} = \frac{\hbar}{2mi} \left(e^{-ik_0z} \vec{\nabla} e^{ik_0z} - e^{ik_0z} \vec{\nabla} e^{-ik_0z} \right) = \frac{\hbar k}{m} \hat{e}_z \quad (2.20)$$

with $\vec{\nabla} = \hat{e}_r \frac{\partial}{\partial r} + \hat{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{e}_\phi \frac{1}{r \sin(\theta)} \frac{\partial}{\partial \phi}$:

$$\vec{j}_{\text{sc}} \stackrel{r \rightarrow \infty}{\equiv} \frac{1}{r^2} |f(\theta, \phi)|^2 \frac{\hbar k}{m} \hat{e}_r + \mathcal{O}\left(\frac{1}{r^3}\right) \quad (2.21)$$

number of particles scattered into direction $d\Omega/\text{sec.}$:

$$n = \vec{j}_{\text{sc}} \cdot \hat{e}_r r^2 d\Omega \quad (2.22)$$

$$\frac{d\sigma}{d\Omega} d\Omega = |f(\theta, \phi)|^2 d\Omega \quad (2.23)$$

$$\frac{d\sigma}{d\Omega} = |f(\theta, \phi)|^2$$

(2.24)

2.2 Propagator theory and the Lippmann-Schwinger equation

As discussed in section 2.1, the scattering problem amounts to the solution of the Schrödinger equation with special, non-trivial boundary conditions for $r \rightarrow \infty$ (namely a plane incoming wave and an angle dependent scattered wave which is solution of the free Schrödinger equation for $r \rightarrow \infty$; $\psi = \psi_{\text{in}} + \psi_{\text{sc}}$).

Therefore, it is useful to separate the problem into

1. a general solution of the Schrödinger equation with open boundary conditions
2. a special solution specifying the appropriate boundary conditions.

This is achieved systematically by the *propagator theory*.

1. General solution

Since we are interested in a stationary scattering problem, we consider the Schrödinger equation fixed energy E . The *resolvent operator* (*Green's operator*) \widehat{G} ("inverse operator") of the Schrödinger operator is defined as the solution of the inhomogeneous Schrödinger equation

$$\boxed{(E - H)\widehat{G} = \mathbb{1}} \quad (\text{representation-free form}) \quad (2.25)$$

with

$$H = H_0 + V, \quad H_0 = \frac{\vec{p}^2}{2m} \text{ free Hamiltonian} \quad (2.26)$$

and

$$V \text{ scattering potential,} \quad \mathbb{1} \text{ unit operator in Hilbert space.} \quad (2.27)$$

Resolvent of the free system \widehat{G}_0 :

$$(E - H_0)\widehat{G}_0 = \mathbb{1} \quad (2.28)$$

The full resolvent \widehat{G} can be expressed in terms of the free resolvent \widehat{G}_0 as follows, separating the perturbation. By multiplying equation (2.25) with \widehat{G}_0 from the left side we get:

$$\boxed{\widehat{G} = \widehat{G}_0 + \widehat{G}_0 V \widehat{G}} \quad (2.29)$$

2. Specific solution $|\psi\rangle$ for the scattering boundary problem:

- (a) $(E - H_0)|\psi\rangle = V|\psi\rangle$
- (b) $(E - H_0)|\phi_0\rangle = 0$ solution of free problem

Subtracting (b) from (a) one obtains:

$$(E - H_0)|\psi\rangle - (E - H_0)|\phi_0\rangle = V|\psi\rangle \quad (2.30)$$

Multiplying with \widehat{G}_0 from the left side we get:

$$|\psi\rangle = |\phi_0\rangle + \widehat{G}_0 V |\psi\rangle \quad (2.31)$$

$$= |\phi_0\rangle + \frac{1}{E - H_0} V |\psi\rangle \quad (2.32)$$

This is the *Lippmann-Schwinger equation*.

Note:

- The free solution $|\phi_0\rangle$ is added in order to account for the plane incoming wave ψ_{in} .
- This equation is very similar to the one describing the time evolution of a state in the context of time-dependent perturbation theory. The only difference is that here we consider the stationary case only. Both are called Lippmann-Schwinger equation.

The equation (2.31) differs from equation (2.29) in that the boundary conditions are implemented via $|\psi_0\rangle$. Equation (2.31) or (2.29) generates a perturbation series for \widehat{G} and $|\psi\rangle$, respectively, via iteration:

$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0 V \widehat{G}_0 + \widehat{G}_0 V \widehat{G}_0 V \widehat{G}_0 + \dots = \quad (2.33)$$

$$\widehat{G} = \widehat{G}_0 + \widehat{G}_0 T \widehat{G}_0 \quad (2.34)$$

$$= \widehat{G}_0 S \widehat{G}_0 \quad (2.35)$$

with

$$T := V + V\widehat{G}_0V + VG_0VG_0V + \dots \quad \text{T-matrix} \quad (2.36)$$

$$S := \widehat{G}_0^{-1} + T \quad (2.37)$$

$$= E - H_0 + T \quad \text{S-matrix} \quad (2.38)$$

Similarly with boundary conditions:

$$|\psi\rangle = |\phi_0\rangle + \widehat{G}_0V|\phi_0\rangle + \widehat{G}_0v\widehat{G}_0V|\phi_0\rangle + \dots \quad (2.39)$$

$$|\psi\rangle = |\phi_0\rangle + \widehat{G}_0T|\phi_0\rangle \quad (2.40)$$

The usefulness of this approach becomes clear when one uses specific representations:

(a) **Momentum representation**

Momentum basis:

$$\left\{ |\vec{p}\rangle = \frac{e^{i\vec{p}\vec{x}}}{\sqrt{2\pi}} \middle| \vec{p} \right\} \quad (2.41)$$

$$\mathbb{1} = \sum_{\vec{p}} |\vec{p}\rangle \langle \vec{p}| = \int \frac{d^3p}{(2\pi)^3} e^{-i\vec{p}\vec{x}} e^{i\vec{p}\vec{x}'} \quad (2.42)$$

$$\mathbb{1} = (E - H_0)G_0 \quad (2.43)$$

$$\Leftrightarrow \langle \vec{p} | \mathbb{1} | \vec{p}' \rangle = \langle \vec{p} | (E - H_0) \sum_{\vec{p}''} |\vec{p}''\rangle \langle \vec{p}'' | G_0 | \vec{p}' \rangle \quad (2.44)$$

$$\underbrace{\delta_{pp'}}_{\text{diagonal}} = \sum_{\vec{p}''} \underbrace{\left(E - \frac{\vec{p}''^2}{2m} \right) \delta_{pp''}}_{\text{diagonal in p-repr.}} \underbrace{G_0}_{=\langle \vec{p}'' | \widehat{G}_0 | \vec{p}' \rangle} \quad (2.45)$$

$$\Rightarrow G_0_{\vec{p}\vec{p}'} = \frac{1}{E - \frac{\vec{p}^2}{2m} \pm i\eta} \delta_{pp'} \quad (2.46)$$

Since \widehat{G}_0 is diagonal in p-representation, it is often identified simply with its diagonal element:

$$G_{0_{\vec{p}}}(E) = \frac{1}{E - \frac{\vec{p}^2}{2m} \pm i\eta} \quad (2.47)$$

The Lippmann-Schwinger equation becomes in p-representation:

$$\langle \vec{p} | \psi \rangle = \langle \vec{p} | \phi_0 \rangle + \int \frac{d^3 p'}{(2\pi)^3} G_{0\vec{p}} V(\vec{p} - \vec{p}') \langle \vec{p}' | \psi \rangle \quad (2.48)$$

with

$$V(\vec{p} - \vec{p}') = \int d^3 x e^{-i(\vec{p} - \vec{p}') \cdot \vec{x}} V(\vec{x}) \quad (2.49)$$

Retarded and advanced Green's functions

From the definition of the resolvent or equation (2.47) it is clear that it has poles as function of E , which require special treatment.

Physical significance of the poles in \widehat{G} :

The position of the poles as function of energy is $E = \epsilon_n =$ energy eigenvalues of H . To treat the poles, e.g. in intergrations over E or \vec{p} they are shifted in the complex E plane away from the real axis by an inifinitesimal positive or negative imaginary part $\pm i\eta$, as indicated above.

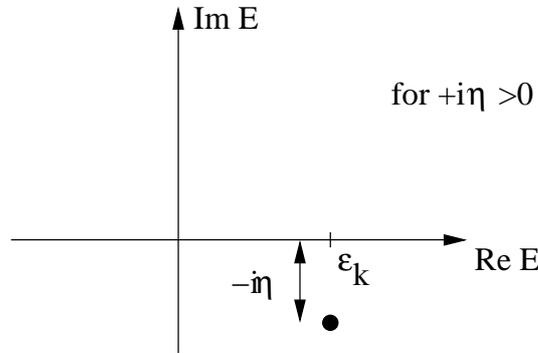


Figure 2.3: Shift of the pole into the complex plane

The relevance of $\pm i\eta$ becomes clear by transforming to the time domain:

Lippmann-Schwinger in time domain

$$\langle \vec{p} | \psi(t) \rangle = \langle \vec{p} | \phi(t) \rangle + \int dt' \int \frac{d^3 p'}{(2\pi)^3} G_{0\vec{p}}(t-t') V(\vec{p} - \vec{p}') \langle \vec{p}' | \psi(t') \rangle \quad (2.50)$$

with the Fourier transform

$$G_{0_{\vec{p}}}(t-t') = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')} G_{0_{\vec{p}}}(\hbar\omega) \quad (2.51)$$

$$= \int \frac{d\omega}{2\pi} \frac{e^{-i\omega(t-t')}}{\hbar\omega - \epsilon_k \pm i\eta} \quad (2.52)$$

$$= \begin{cases} -i\theta(t-t') e^{-\frac{i}{\hbar}\epsilon_k(t-t')}, & +i\eta \\ i\theta(t-t') e^{-\frac{i}{\hbar}\epsilon_k(t-t')}, & -i\eta \end{cases} \quad (2.53)$$

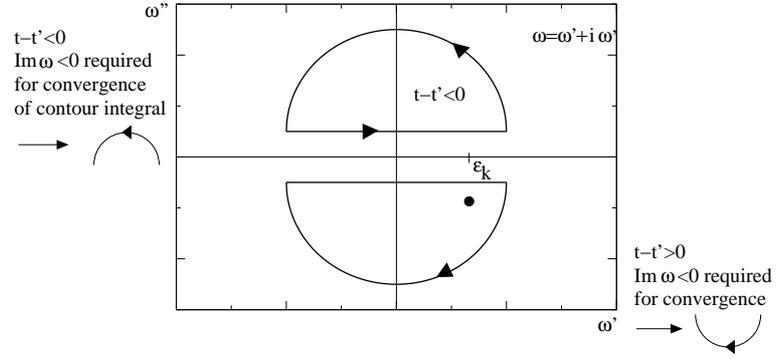


Figure 2.4: Contour integration

$$\langle \vec{p} | \psi(t) \rangle = \langle \vec{p} | \phi(t) \rangle + \int_{-\infty}^{\infty} dt' \int \frac{d^3 p'}{(2\pi)^3} G_{0_{\vec{p}}}^{r/a}(t-t') V(\vec{p}-\vec{p}') \langle \vec{p}' | \psi(t') \rangle \quad (2.54)$$

$G^{r/a}$ is called the retarded/advanced propagator, because it propagates the wave function t' to t with $t > t'$ (retarded, causal), $t < t'$ (advanced, acausal).

(b) **Position representation**

$$\psi(x) = \langle x | \psi \rangle \quad \text{etc.} \quad \text{fixed energy } E \quad (2.55)$$

$$\psi(x) = \phi_0(x) + \int d^3 x' G_0(\vec{x}, \vec{x}') V(\vec{x}') \psi(\vec{x}') \quad (2.56)$$

$$G_0^{r,a}(\vec{x}, \vec{x}') = \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} G_{0\vec{p}}^{r,a}(E) \delta_{\vec{p}\vec{p}'} e^{\frac{i}{\hbar}\vec{p}\vec{x}} e^{\frac{i}{\hbar}\vec{p}'\vec{x}'} \quad (2.57)$$

$$= \langle \vec{x} | \widehat{G}_0^{r,a} | \vec{x}' \rangle \quad \vec{k} = \frac{\vec{p}}{\hbar} \quad (2.58)$$

$$G_0^{r,a}(\vec{x}, \vec{x}') = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{e^{\pm i\vec{k}|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|} \quad (2.59)$$

$$\text{with } \vec{k} = \sqrt{\frac{2mE}{\hbar^2}} \quad (2.60)$$

Interpretation of the Lippmann-Schwinger equation and its expansion in terms of Feynman diagrams:

$$G = G_0 + \int dx'' G_0(x, x'') V(x'') G_0(x'', x') \quad (2.61)$$

$$= \dots \quad (2.62)$$

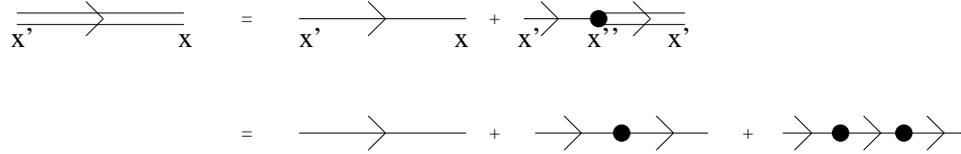


Figure 2.5: L-S equation in terms of Feynman diagrams

The scattering amplitude $f(\theta, \phi)$:

From (2.56) in the limit $|\vec{x}| \gg |\vec{x}'|$ we can now identify the scattering amplitude.

Choose:

$$\phi_0(x) = \psi_{\text{in}} = e^{ikz}, \quad k = \sqrt{\frac{2mE}{\hbar^2}} \quad (2.63)$$

Since the potential $V(\vec{x}')$ is localized in space, the \vec{x}' integral in (2.56) runs over a region $|\vec{x}'| \lesssim r_0$, i.e. we can take the limit $|\vec{x}| \gg |\vec{x}'|$ with

$r = |\vec{x}|$ and $\vec{k}' = k = \vec{k}_{\text{out}}$:

$$G_0^{r,a}(\vec{x} - \vec{x}') \underset{\vec{x} \rightarrow \infty}{\cong} -\frac{1}{4\pi} \frac{2m}{\hbar^2} \underbrace{\frac{e^{(\pm)ikr}}{r}}_{\text{only outgoing parts}} e^{(\mp)i\vec{k}'\vec{x}'} \quad (2.64)$$

$$\begin{aligned} \psi(\vec{x}) &= e^{ikz} + \left[-\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' e^{-i\vec{k}\vec{x}'} V(\vec{x}') \right. \\ &\quad \left. \times \psi(\vec{x}') \right] \frac{e^{ikr}}{r} \end{aligned} \quad (2.65)$$

$$\begin{aligned} &= e^{ikz} + \left[-\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' e^{-i\vec{k}'_{\text{out}}\vec{x}'} \right. \\ &\quad \left. \times T(\vec{x}', \vec{x}') \underbrace{e^{i\vec{k}_{\text{in}}\vec{x}'}}_{\phi_0(\vec{x}')} \right] \frac{e^{ikr}}{r} \end{aligned} \quad (2.66)$$

$$f(\theta, \phi) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' e^{-i(\vec{k}_{\text{out}} - \vec{k}_{\text{in}})\vec{x}'} T(\vec{x}', \vec{x}') \quad (2.67)$$

$$f(\vec{k}_{\text{out}}, \vec{k}_{\text{in}}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 T(\vec{k}_{\text{out}}, \vec{k}_{\text{in}}) \quad (2.68)$$

Born approximation:

Iterate the Lippmann-Schwinger equation only once. Replace $T(\vec{k}_{\text{out}}, \vec{k}_{\text{in}})$ by $V(\vec{k}_{\text{out}} - \vec{k}_{\text{in}})$ in all expressions above.

Expansion:

$$k|\vec{x} - \vec{x}'| \cong \vec{k}'\vec{r} - \underbrace{k\vec{x}}_{\vec{k}' = \vec{k}_{\text{out}}} \cdot \vec{x}' \quad (2.69)$$

2.3 The optical theorem

Relation between the imaginary part of the forward scattering amplitude $\text{Im } f(\theta = 0)$ and the total cross section $\sigma_{\text{tot}} = \int d\Omega \frac{d\sigma}{d\Omega}$.

$$\text{Im } f(\theta = 0) = \frac{k}{4\pi} \sigma_{\text{tot}} \quad k = \sqrt{\frac{2mE}{\hbar^2}} \quad (2.70)$$

Proof: $G^a = (G^r)^*$

$$f(\theta = 0) = f(\vec{k}, \vec{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \vec{k} | T | \vec{k} \rangle \quad (2.71)$$

$$\text{Im} \langle \vec{k} | T | \vec{k} \rangle = \text{Im} \langle \vec{k} | V | \psi \rangle \quad (2.72)$$

$$= \text{Im} [(\langle \psi | - \langle \psi | V G_0^a V | \psi \rangle)] \quad (2.73)$$

$$= \text{Im} [\underbrace{\langle \psi | V | \psi \rangle}_{\text{real}} - i\pi \langle \psi | V \delta(E - H_0) V | \psi \rangle] \quad (2.74)$$

$$= -\pi \langle \psi | V \delta(E - H_0) V | \psi \rangle \quad (2.75)$$

$$= -\pi \langle \vec{k} | T^+ \delta(E - H_0) T | \vec{k} \rangle \quad (2.76)$$

$$= -\pi \int d^3k \langle \vec{k} | T^+ | \vec{k}' \rangle \langle \vec{k}' | T | \vec{k} \rangle \delta\left(E - \frac{\hbar^2 k}{2m}\right) \quad (2.77)$$

$$= -\pi \int d\Omega \frac{mk}{\hbar^2} |\langle \vec{k}' | T | \vec{k} \rangle|^2 \quad (2.78)$$

2.3.1 Partial wave expansion: scattering phase shift

In section 2.1 we had seen that in the far-field region, $|\vec{r}| \gg r_0$ (where $r_0 =$ extension of the potential $V(\vec{r}) \approx 0$, $|\vec{r}| > r_0$), the scattered wave is a *radially outgoing* wave, with an angle-dependent outgoing current density:

$$\psi(\vec{r}) \underset{r \gg r_0}{=} e^{i\vec{k}\vec{r}} + f(\theta, \phi) \frac{e^{ikr}}{r} = \psi_{\text{in}} + \psi_{\text{sc}} \quad (2.79)$$

$$\vec{j}_{\text{sc}}(\theta, \phi) = \frac{\hbar k}{m} |f(\theta, \phi)|^2 \frac{\hat{e}_r}{r^2} + \mathcal{O}\left(\frac{1}{r^3}\right) \quad (2.80)$$

For $|\vec{r}| > r_0$, $\psi_{\text{sc}}(\vec{r})$ is a solution of the free Schrödinger equation, which separates into angular momentum and radial parts. We could, therefore, write ψ_{sc} as an expansion in the complete set of spherical harmonics

$$\psi_{\text{sc}}(r \rightarrow \infty, \theta, \phi) = \sum_{l,m} [A_l j_l(k_0 r) + B_l n_l(k_0 r)] Y_l^m(\theta, \phi) \quad (2.81)$$

where the expansion coefficients $[A_l j_l(k_0 r) + B_l n_l(k_0 r)]$ are the general solution of the radial Schrödinger equation

$$\left(-\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{l(l+1)}{r^2} \right) R(r) = k_0 R(\vec{r}), \quad k_0 = \sqrt{2mE/\hbar^2} \quad (2.82)$$

and the coefficients A_l, B_l are to be determined such that $\psi_{\text{sc}}(r)$ equation (2.67) crosses over smoothly to the solution in the near-field region of the potential, $r \lesssim r_0$. The coefficients C_l of the expansion do not depend on m , since the radial Schrödinger equation does not for a spherical potential. From the requirement that ψ_{sc} contains only outgoing waves (and the asymptotic behavior of $j_l(k_0 r), n_l(k_0 r)$ for $r \rightarrow \infty$) we obtained $A_l = -iB_l$ and

$$f(\theta, \phi) = \sum_l \frac{1}{k_0} (-i)^{l+1} B_l(k_0) Y_l^0(\theta, \phi) \quad (2.83)$$

$$=: \sum_l (2l+1) f_l(k_0) \mathcal{P}_l(\cos(\theta)). \quad (2.84)$$

The expansion coefficients f_l of the expansion of $f(\theta, \phi)$ are called *partial wave amplitudes* $f_l(k_0)$ (independent of m). In order to get a complete understanding of the scattering process in terms of the partial waves Y_l^m , i.e. angular momentum channels l, m , it is also useful to expand the incoming plane wave ψ_{in} in terms of spherical harmonics and Bessel functions. This can be done, because $\psi_{\text{in}}(\vec{r}) = e^{i\vec{k}_0 \vec{r}}$ is a solution of the free Schrödinger equation for energy $E = \frac{\hbar^2 k_0^2}{2m}$ and $\{j_l(k_0 r) Y_l^m(\theta, \phi), n_l(k_0 r) Y_l^m(\theta, \phi) | l = 0, 1, \dots, m = -l, \dots, +l\}$ is a complete basis set of solutions of the free Schrödinger equation for energy $E = \frac{\hbar^2 k_0^2}{2m}$ as well.

One obtains:

$$e^{i\vec{k}_0 \vec{r}} = \sum_l i^l (2l+1) j_l(k_0 r) Y_l^0(\theta, \phi) \quad (2.85)$$

$$= \sum_{l=1}^{\infty} i^l (2l+1) j_l(k_0 r) \underbrace{\mathcal{P}_l(\widehat{k}_0 \cdot \widehat{r})}_{\cos(\theta)} \quad (2.86)$$

- Only the $m = 0$ component contributes, because $e^{i\vec{k}_0 \vec{r}}$ is cylindrically symmetric about \vec{k}_0 axis.
- The von Neumann functions $n_l(k_0 r)$ do not contribute, because they are singular for $\vec{r} = 0$.

- Expansion coefficients (with proper normalization):

$$\left\langle E = \frac{\hbar^2 k_0^2}{2m}, l, m \left| \vec{k}_0 \right. \right\rangle = \int d^3r E = \frac{\hbar^2 k_0^2}{2m}, l, m \underbrace{|\vec{r}\rangle \langle \vec{r}|}_{=1} \vec{k}_0 \rangle \quad (2.87)$$

$$= \int d^3r k_0^3 j_l(k_0 r) (Y_l^0(\theta, \phi))^* \cdot e^{i\vec{k}_0 \vec{r}} \quad (2.88)$$

$$= \int_0^\infty dr r^2 k_0^3 \underbrace{\int_0^{2\pi} d\phi \int_{-1}^{+1} d \cos(\theta)}_{\rightarrow \delta_{m0}} j_l(k_0 r) P_l(\cos(\theta)) e^{i\vec{k}_0 \cos(\theta)} \quad (2.89)$$

$$\times e^{-im\phi} P_l(\cos(\theta)) e^{i\vec{k}_0 \cos(\theta)} \quad (2.90)$$

$$= i^l (2l + 1) \quad (2.90)$$

Hence, we have for the complete solution of the scattering problem of a spherically symmetric potential:

scattering amplitude $f(\theta, \phi) = f(\theta)$ independent of ϕ and

$$\psi(\vec{r}) \stackrel{r \rightarrow \infty}{\equiv} e^{i\vec{k}_0 \vec{r}} + f(\theta) \frac{e^{i\vec{k}_0 \vec{r}}}{r} \quad (2.91)$$

$$\psi(\vec{r}) \stackrel{r \rightarrow \infty}{\equiv} \sum_l \left[(2l + 1) P_l(\cos(\theta)) e^{il\frac{\pi}{2}} \frac{e^{i(k_0 r - l\frac{\pi}{2})} - e^{-i(k_0 r - l\frac{\pi}{2})}}{2ik_0 r} \right. \quad (2.92)$$

$$\left. + (2l + 1) f_l(k_0) P_l(\cos(\theta)) \frac{e^{ikr}}{r} \right]$$

The first summand is a plane wave and the second one is the scattered wave ψ_{sc} .

Interpretation:

- The incoming plane wave consists of incoming and outgoing spherical harmonics $\equiv \frac{e^{-ik_0 r}}{r}, \equiv \frac{e^{+ik_0 r}}{r}$.
- The effect of the scattering potential is to change the amplitude of the outgoing wave.

$$1 \longrightarrow 1 + 2ik_0 f_k(k_0) \quad (2.93)$$

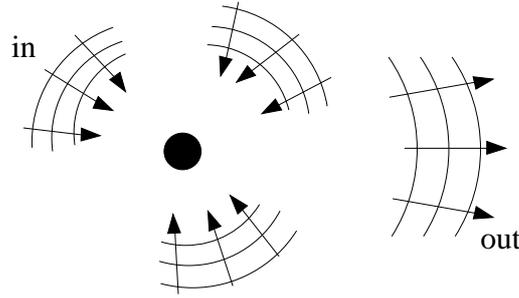


Figure 2.6:

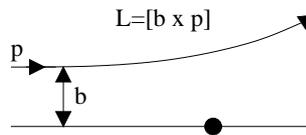


Figure 2.7: Change of the amplitude

- The incoming plane wave consists of many different angular momentum contributions, like in the classical case $|\vec{L}| = b \cdot |\vec{p}|$ (arbitrary impact parameter b), but $|\vec{L}|^2$ quantized in quantum case. Each l channel has different scattering amplitude f_l .
- The current conservation (in the case of scattering without absorption or emission) implies:

$$\vec{\nabla} \cdot \vec{j}^{\text{continuity}} - \frac{\partial}{\partial t} |\psi|^2 = 0 \quad (2.94)$$

(no current source or sink; inward/outward going currents are equal)

Hence the incoming and outgoing currents must be equal and opposite.
Orthogonality of the partial waves \Rightarrow

$$S_l := (1 + 2ik_0 f_l(k_0)) \quad (2.95)$$

with

$$|S_l|^2 = 1 \quad (2.96)$$

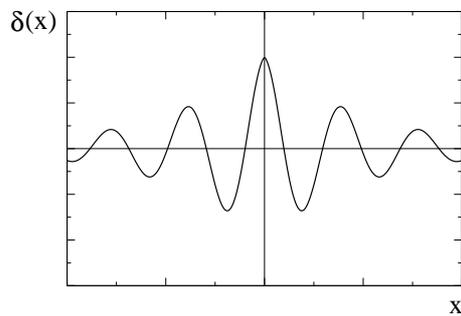


Figure 2.8:

- **Scattering phase shift:**

The imaginary part in S_l implies that the scattered outgoing wave acquires a phase shift $2\delta_l$ compared to the incoming wave (with $|S_l| = 1$):

$$S_l = e^{2i\delta_l} = 1 + 2ik_0 f_l \quad (2.97)$$

or

$$f_l = \frac{e^{2i\delta_l} - 1}{2ik_0} = \frac{1}{k_0} e^{i\delta_l} \sin(\delta_l) \quad (2.98)$$

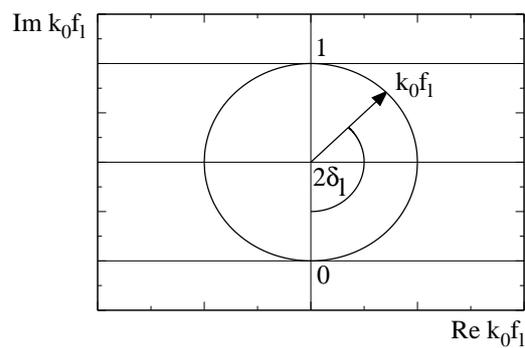


Figure 2.9:

Hence, the total scattering amplitude can be expressed in terms of the

partial scattering phase shifts:

$$f(\theta) = \frac{1}{k_0} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin(\delta_l) P_l(\cos(\theta)) \quad (2.99)$$

$$= \sum_{l=0}^{\infty} (2l+1) f_l(k_0) P_l(\cos(\theta)) \quad (2.100)$$

2.3.2 The optical theorem

This result confirms the optical theorem:

$$\text{Im } f(\theta = 0) = \sum_{l=0}^{\infty} \frac{2l+1}{k_0} \text{Im} (e^{i\delta_l}) \cdot \sin(\delta_l) P_l(1) \quad (2.101)$$

$$= \sum_l \frac{2l+1}{k_0} \sin^2(\delta_l) \quad (2.102)$$

$$(2.103)$$

$$\sigma_{\text{tot}} = \int d\Omega |f(\theta)|^2 \quad (2.104)$$

$$= \frac{2\pi}{k_0^2} \int_{-1}^{+1} d \cos(\theta) \sum_{l,l'} (2l+1)(2l'+1) e^{i(\delta_l - \delta_{l'})} \quad (2.105)$$

$$\times \sin(\delta_l) \sin(\delta_{l'})$$

$$\times P_l(\cos(\theta)) P_{l'}(\cos(\theta))$$

$$\stackrel{(*)}{=} \frac{4\pi}{k_0^2} \sum_l (2l+1) \sin^2(\delta_l) \quad (2.106)$$

$$(*) \int_{-1}^{+1} d \cos(\theta) (2l+1) P_l(\cos(\theta)) P_{l'}(\cos(\theta)) = \delta_{ll'} \quad (2.107)$$

$$\rightarrow \boxed{\text{Im } f(\theta = 0) = \frac{k_0}{4\pi} \sigma_{\text{tot}}} \quad (2.108)$$

It is seen from the above considerations, that the scattering problem is solved, once the phase shifts are known.

2.3.3 Determining the scattering phase shifts for an arbitrary potential

The coefficients of the partial wave expansion in the outside region ($|\vec{r}| > r_0$) are determined by matching the outside solution of the radial Schrödinger equation for given l to the inside solution. Therefore, we seek an explicit expression of the δ_l in terms of the radial solutions:

Total wave function at any $|\vec{r}| > r_0$ (spherical potential):

$$\psi(\vec{r}) = \sum i^l (2l + 1) A_l(r) P_l(\cos(\theta)) \quad (2.109)$$

$A_l(r)$ solution of the radial Schrödinger equation with potential:

$$\left[-\frac{1}{r^2} \frac{\partial}{\partial r^2} r^2 \frac{\partial}{\partial r^2} + \frac{l(l+1)}{r^2} + \frac{2m}{\hbar^2} V(r) \right] A_l(r) = k_0^2 A_l(r) \quad (2.110)$$

or with $u_l = r A_l(r)$:

$$\frac{d^2 u_l}{dr^2} + \left(k_0^2 - \frac{2m}{\hbar^2} V(r) - \frac{l(l+1)}{r^2} \right) u_l = 0 \quad (2.111)$$

A_l with boundary condition $u_l(r=0) = 0$ as in hydrogen problem.

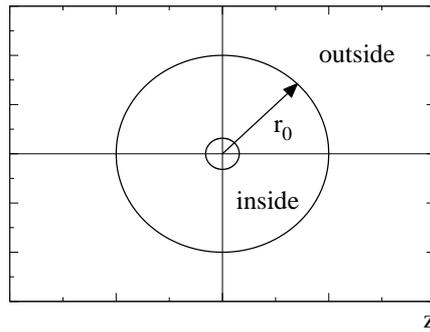


Figure 2.10:

Matching (2.80) with (2.72) and (2.78) for $r \gg r_0$ yields with $A_l(r) = a_1 j_l + a_2 n_l$:

$$A_l(r) = e^{i\delta_l} [\cos(\delta_l) j_l(k_0 r) - \sin(\delta_l) n_l(k_0 r)] \quad (2.112)$$

Solution by logarithmic derivative:

$$\beta_l \equiv \frac{r}{A_l} \frac{dA_l}{dr} \Big|_{r=r_0} \quad \text{condition on } r_0: V(r_0) \approx 0 \quad (2.113)$$

$$= kr_0 \left[\frac{j_l'(k_0 r_0) \cos(\delta_l) - n_l'(k_0 r_0) \sin(\delta_l)}{j_l(k_0 r_0) \cos(\delta_l) - n_l(k_0 r_0) \sin(\delta_l)} \right] \quad (2.114)$$

$$\leadsto \tan(\delta_l) = \frac{kr_0 j_l'(k_0 r_0) - \beta_l j_l(k_0 r_0)}{kr_0 n_l'(k_0 r_0) - \beta_l n_l(k_0 r_0)} \quad (2.115)$$

Solve for $A_l(r_0)$ by integrating radial Schrödinger equation.

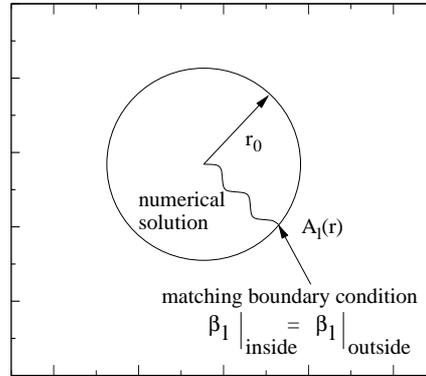


Figure 2.11:

2.3.4 Scattering at low energies and bound states

r_0 = range of the scattering potential

At low energies, i.e. for $\lambda = \frac{2\pi}{k_0} > r_0$, partial waves with $l > 0$ are in general unimportant:

Total potential in angular momentum channel l :

$$V_{\text{eff}} = V(r) + \underbrace{\frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}}_{V_{\text{cf},l}(r)} \quad (2.116)$$

- Classically for $l > 0$ the particle cannot penetrate the centrifugal potential, so that it does not "feel" the potential $V(r)$ inside the centrifugal barrier.

Classical estimate:

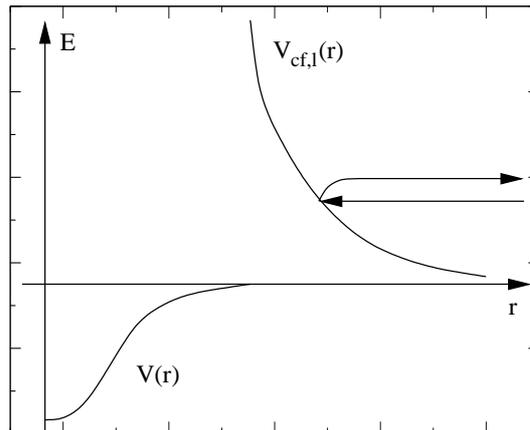


Figure 2.12:

In order to feel the potential of range r_0 inside, it must penetrate the barrier at least down to r_0 , i.e. it must have at least the energy

$$E = \frac{\hbar^2 k_0^2}{2m} \geq \frac{\hbar^2 l(l+1)}{2m r_0^2} \quad (2.117)$$

$$\Rightarrow \lambda = \frac{2\pi}{k_0} \leq \frac{2\pi r_0}{\sqrt{l(l+1)}}, \quad (2.118)$$

where λ is the wave length of the incident particle.

- Quantum mechanically, the scattering phase δ_l and, hence, $f_l(k_0)$ vanishes as:

$$\delta_l \sim k_0^{2l+1} \quad (2.119)$$

The scattering length a

Rectangular potential well, to be specific:

$$V(r) = \begin{cases} V_0 = \text{const.} & r < r_0 & V_0 > 0 \text{ repulsive} \\ 0 & r \geq 0 & V_0 < 0 \text{ attractive} \end{cases} \quad (2.120)$$

k_0 : incident wave number

We consider s-wave scattering only (low energy):

- $r > r_0$:

$$A_{l=0}(r) = e^{i\delta_l} [\cos(\delta_l) j_l(k_0 r) - \sin(\delta_l) n_l(k_0 r)] \Big|_{l=0} \quad (2.121)$$

$$\stackrel{\cong}{\underset{r \rightarrow \infty}{}} e^{i\delta_l} \frac{\sin(k_0 r - l\pi + \delta_l)}{k_0 r} \Big|_{l=0} \quad (2.122)$$

$$= e^{i\delta_l} \frac{\sin(k_0 r + \delta_l)}{k_0 r} \quad (2.123)$$

Here we have used:

$$j_{l=0}(k_0 r) = \frac{\sin(k_0 r - l\pi)}{k_0 r} \quad (2.124)$$

$$n_{l=0}(k_0 r) = \frac{\cos(k_0 r - l\pi)}{k_0 r} \quad (2.125)$$

$$\sin(a \pm b) = \sin(a) \cos(b) \pm \cos(a) \sin(b) \quad (2.126)$$

- $r < r_0$:

$$u(r) \equiv r A_{l=0}(r) \sim \sin(k' r) \quad (2.127)$$

with $E - V_0 = \frac{\hbar^2 k'^2}{2m}$ for $V = \text{const.}$

Radial Schrödinger equation

$$\frac{d^2 u}{dr^2} + \left(k'^2 - \frac{2m}{\hbar^2} V_0 \right) u = 0 \quad (l = 0) \quad (2.128)$$

and boundary condition $u(r = 0) = 0$.

For $E - V_0 > 0$ inside solution has same form as outside solution, but for

$$V_0 < 0 \quad k' > k_0 \quad \text{attractive} \quad (2.129)$$

$$V > 0 \quad k' < k_0 \quad \text{repulsive} \quad (2.130)$$

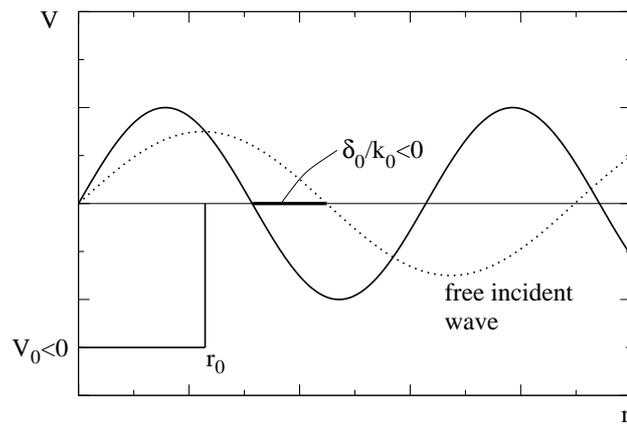


Figure 2.13: V_0 attractive

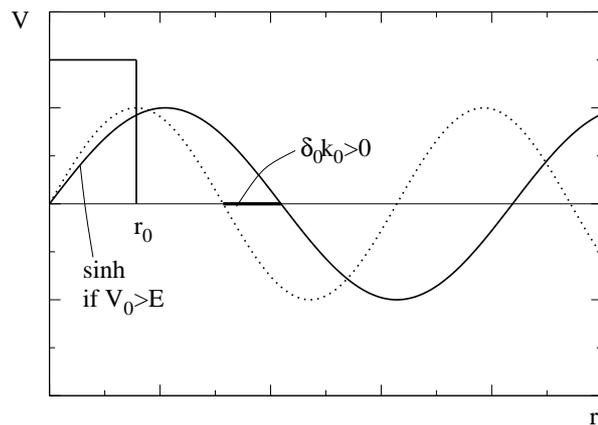


Figure 2.14: V_0 repulsive

Ramsauer-Townsend effect

$$V_0 < 0, \quad \lambda = \frac{2\pi}{k_0} \gg r_0, \quad \boxed{k_0 r_0 \ll 1} \quad (2.131)$$

(1.) $V_0 < 0$ such that $(k' r_0) = \frac{\pi}{2}, \delta_0 \cong \frac{\pi}{2}$

→ marginal cross section in $l = 0$ channel:

$$\hat{\sigma}_{0,\text{tot}} = |f_l|^2 = \frac{1}{k_0^2} \sin^2(\delta_0) = \frac{1}{k_0^2} \quad (2.132)$$

(2.) $V_0 < 0$ such that $(k' r_0) = \pi, \delta_0 = \pi$ but total cross section $\sigma_{0,\text{tot}} \approx 0!$

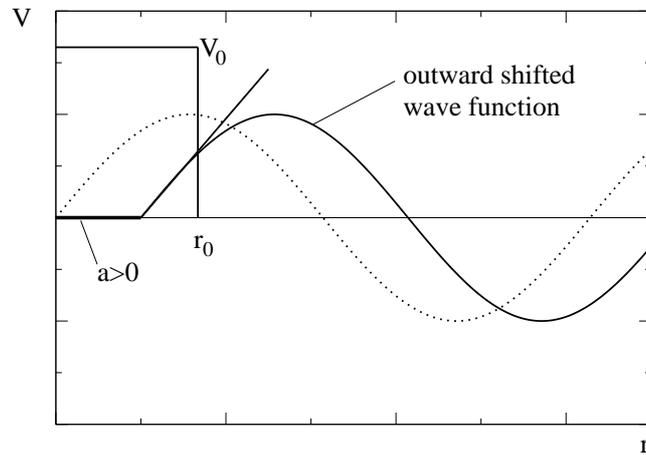
The scattering length

Figure 2.15: The scattering length

a : scattering length: x-axis intercept of the linear extrapolation of the outside wave function to $\psi = 0$

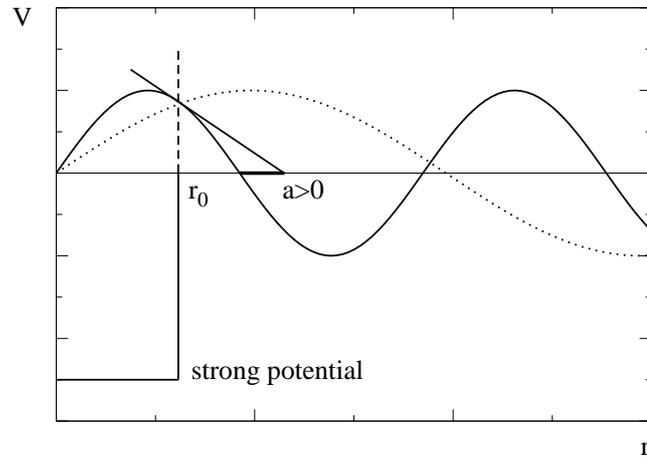


Figure 2.16:

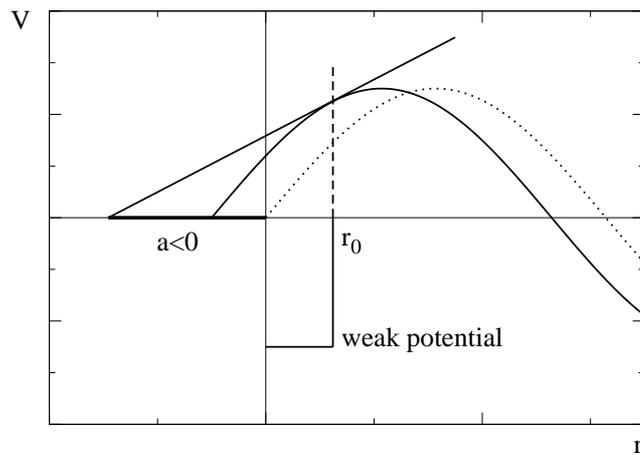


Figure 2.17:

Relation between binding energy and a when there is a bound state

$$\kappa \approx \frac{1}{a}, \quad \kappa = \sqrt{-\frac{2m(V_0 - E_B)}{\hbar^2}}, \quad f_l = -a \quad (2.133)$$

This result can be obtained in a pure fundamental way from the analytical structure of $S_l(k_0)$ in the complex k_0 plane.

2.3.5 Bound states as poles of $S_l(k_0)$ at low energies

$$S_l(k_0) = 1 + 2ik_0 f_l(k_0) = e^{2i\delta_l} \quad (2.134)$$

s-wave scattering only, $V_0 < 0$

$r \gg r_0$:

$$A_0(r) \sim \left[S_{l=0}(k_0) \frac{e^{ik_0 r}}{r} - \frac{e^{-ik_0 r}}{r} \right] \quad (2.135)$$

Bound state wave function:

$r \gg r_0$:

$$\widehat{A}_0(r) \sim \frac{e^{-\kappa r}}{r} \quad \text{with } E < 0 \quad (2.136)$$

with imaginary wave number $k_0 = i\kappa$ ("outward going")

Consider $S_{l=0}(k_0)$ as function of *complex* k_0 and investigate analytical structure (if we have no further information then bound states). For bound state wave function no ingoing wave ($\sim e^{+\kappa r}$) possible. For normalized bound state wave function, S is the ratio between outward and inward going contributions.

$\rightarrow S_{l=0}(k_0 = i\kappa) \rightarrow \infty$ must have *pole*.

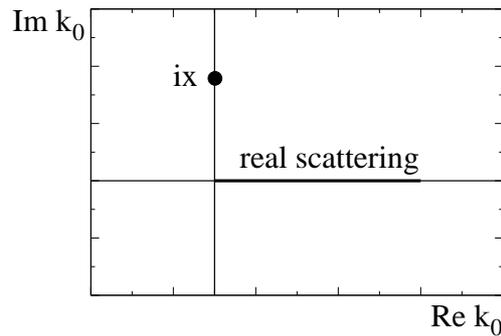


Figure 2.18:

General properties of $S_0(k_0)$:

- (1.) Pole at $k = i\kappa$ (bound state)
- (2.) $|S_{l=0}| = 1, k > 0$ (unitarity)
- (3.) $S_{l=0} = e^{2i\delta_0} = 1$ for $k \rightarrow 0$ (since $\delta_0 \rightarrow 0$)

Construct analytical function everywhere except $k_0 = i\kappa$.

$$S_{l=0}(k_0) = \frac{-k_0 - i\kappa}{k_0 - i\kappa} \quad (\text{Pade approximation}) \quad (2.137)$$

(may be generalized for more bound states: poles in *upper* half complex plane)

$$f_{l=0} = \frac{S_{l=0} - 1}{2ik_0} \stackrel{\text{Pade}}{=} \frac{1}{-\kappa - ik_0} \quad (2.138)$$

$k_0 \rightarrow 0$:

$$\frac{1}{-\kappa} \rightarrow f_{l=0} = -a \quad (2.139)$$

2.3.6 Resonance scattering

Resonant effects occur (like in any physical system) if the energy (frequency) of the incoming wave coincides with the energy $E_0 = \frac{\hbar^2 k_0^2}{2m}$ of a (discrete) bound state of the scattering potential. Since $E_0 > 0$, this is possible, if the "bound state" energy is positive, i.e. the potential must have the form:

quasibound state: tunneling to the outside region possible

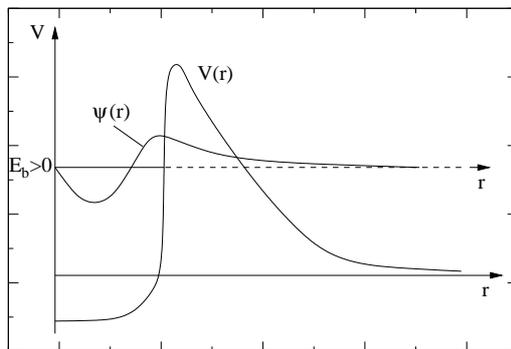


Figure 2.19:

The potential must have an attractive inside region and a confining, repulsive well in some finite range for $r > 0$. Since $V(r) \xrightarrow{r \rightarrow \infty} 0$, tunneling from the discrete state at $E_b > 0$ inside the potential to the free outside states at *the same* energy is possible \rightarrow quasibound state.

This situation is generically realized by a sufficiently strong, nondivergent, attractive potential $V(r)$ in angular momentum channels $l \geq 1$, because of the centrifugal potential $\frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} = V_{\text{cf}}$.

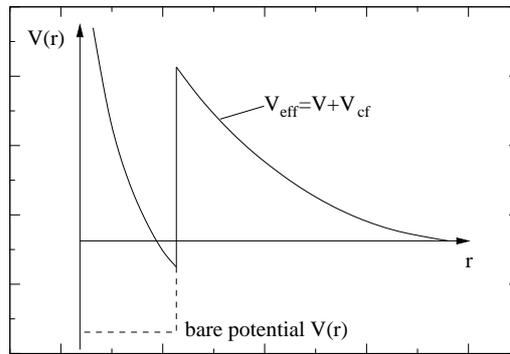


Figure 2.20:

Energy dependence of the scattering cross section

(in angular momentum channel l)

In general the scattering phase shift $\delta_l(E)$ has a smooth energy dependence ($E = \frac{\hbar^2 k_0^2}{2m}$).

\rightarrow The scattering cross section in channel l

$$\sigma_t = |f_l|^2 \cdot \underbrace{4\pi(2l+1)}_{\int d\Omega, \text{prefactor } 2l+1}, \quad f_l = e^{i\delta_l(k_0)} \frac{\sin(\delta_l(k_0))}{k_0} \quad (2.140)$$

varies smoothly with energy.

From the expression for f_l it follows that σ_l has a maximum for $\delta_l = \frac{\pi}{2} + n\pi, n \in \mathbb{Z}$.

\rightarrow resonant behavior for $E = E_r, k_0 = k_r$

The resonant energy $E_r \approx E_b$

Shape of the scattering amplitude $f_l(k_0)$ near $k_0 = k_r$:

$\delta_l(k_0)$ continuous near $k_0 = k_r$, $\delta_l(k_r) = \frac{\pi}{2}$.

Expand f_l about k_r, E_r :

$$f_l(E) = \frac{e^{2i\delta_l} - 1}{2ik_0} \quad (2.141)$$

$$= \frac{e^{i\delta_l} \sin(\delta_l)}{k_0} \quad (2.142)$$

$$= \frac{1}{k_0} \frac{\sin(\delta_l)}{\cos(\delta_l) - i \sin(\delta_l)} \quad (2.143)$$

$$= \frac{1}{k_0} \frac{1}{\cot(\delta_l) - i} \quad (2.144)$$

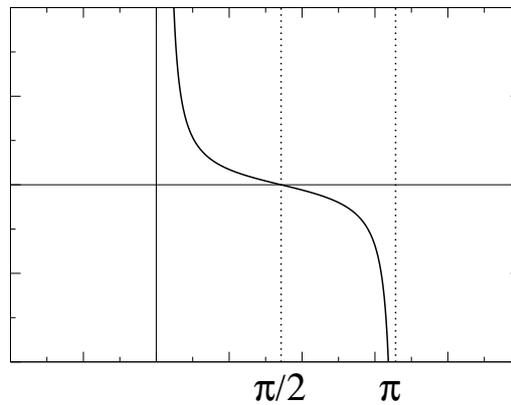


Figure 2.21:

$$\cot(\delta_l) = \underbrace{\cot(\delta_l(E))\Big|_{E=E_r}}_{=0} + \frac{d \cot(\delta_l)}{dE}\Big|_{E=E_r} (E - E_r) + \mathcal{O}[(E - E_r)^2] \quad (2.145)$$

$$\cong -\frac{2}{\Gamma}(E - E_r) \quad \left[-\frac{2}{\Gamma} = \frac{d \cot(\delta_l)}{dE} \right] \quad (2.146)$$

$$f_l(E) = -\frac{1}{\underbrace{\sqrt{2mE/\hbar^2}}_{k_0}} \frac{\Gamma/2}{(E - E_r) + i\frac{\Gamma}{2}} \quad (2.147)$$

$$\sigma_l(E) = 4\pi \cdot (2l + 1) |f_l|^2 \quad (2.148)$$

$$= \frac{4\pi}{k_0^2} \frac{(\Gamma/2)^2}{(E - E_r)^2 + \Gamma^2/4} \quad (2.149)$$

Scattering amplitude:

$$f_l = f_l' + i f_l'' \quad (2.150)$$

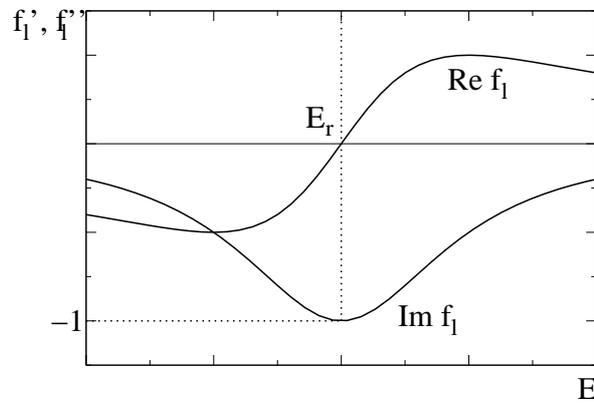


Figure 2.22:

$$f_l(E) \cong \frac{1}{k_0} \frac{\Gamma/2(E - E_r) - i(\Gamma/2)^2}{(E - E_r)^2 + (\Gamma/2)^2} \quad (2.151)$$

Γ =full width at half maximum (FWHM)

Cross section:

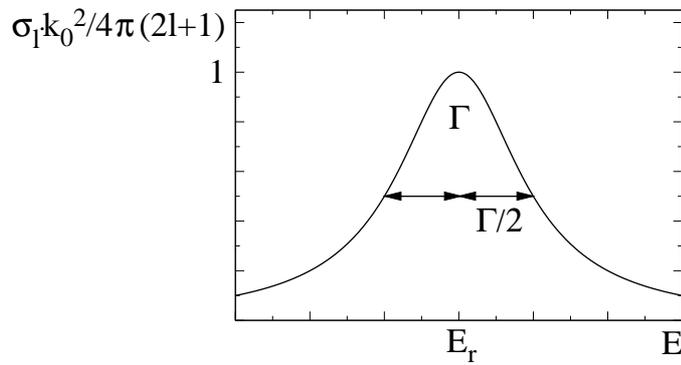


Figure 2.23:

from $f_l = e^{i\delta_l} \frac{\sin(\delta_l)}{k_0}$:

$$\tan(\delta_l) = \frac{\sin(\delta_l)}{\cos(\delta_l)} = \frac{\text{Im}(f_l)}{\text{Re}(f_l)} = \frac{-\Gamma/2}{E - E_r} \quad (2.152)$$

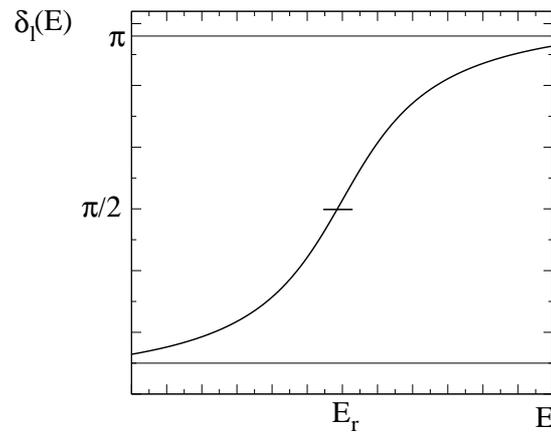


Figure 2.24:

2.3.7 The Friedel sum rule

Scattering potential (charge Ze) immersed into an electron sea, filled up to Fermi wave number k_F due to Pauli principle.

→ Complete screening of the charge by the surrounding electrons.

The charge Ze can be expressed in terms of the scattering phase shifts of the electron wave functions in the presence of the potential. We assume a spherical electron sea with charge in the center and radius R .

Without charge:

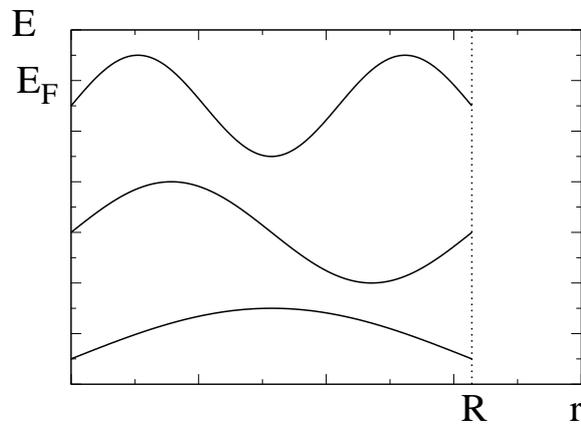


Figure 2.25:

The radial wave functions *without* the scattering potential are the Bessel functions (regular for $r \rightarrow 0$)

$$j_l(kr) \stackrel{r \rightarrow \infty}{\equiv} \frac{1}{kr} \sin\left(kr - l\frac{\pi}{2}\right) \quad (2.153)$$

with boundary condition $j_l(kR) = 0$ at $r = R$, i.e. quantized wave numbers:

$$k_n R = \left(n - \frac{l}{2}\right) \pi \quad (2.154)$$

For $R \rightarrow \infty$ k_n becomes quasi-continuous.

In the presence of the charge Ze the solutions are for $r \rightarrow \infty$:

$$C_l \frac{1}{kr} \sin\left(kr + \delta_l - \frac{l\pi}{2}\right) \quad (2.155)$$

because of the scattering amplitude $f_l = \frac{1}{k_0} e^{i\delta_l} \sin(\delta_l)$, and scattered wave function $\sim f_l \frac{e^{i(kr-l\pi/2)}}{r}$.

Quantized momenta:

$$k_n R + \delta_l = \left(n + \frac{l}{2} \right) \pi \quad (2.156)$$

For each n , there is a particle state k_n , which is filled with electron up to $E(k_n) = E_F$ (Fermi). Thus, the presence of the potential changes the number of occupied electron states because of the phase shifts δ_l , i.e. the number of electrons in the volume R .

This change of e^- number must be equal to $\Delta n = Z$, the charge number of the impurity (charge neutrality).

We count this change of particle number:

Number of states in $[k, k + dk]$ (with charge)

$$dn = \frac{dn}{dk} dk = \left(\frac{R}{\pi} + \frac{1}{\pi} \frac{\partial \delta_l}{\partial k} \right) dk \quad (2.157)$$

Number of states in $[k, k + dk]$ (without charge)

$$dn_0 = \frac{dn_0}{dk} dk = \frac{R}{\pi} dk \quad (2.158)$$

$$\Delta(dn) = dn - dn_0 = \frac{1}{\pi} \frac{\partial \delta_l}{\partial k} dk \quad (2.159)$$

→ Total change in number of states in $[k, k + dk]$ for *all* channels (including spin):

$$\frac{d}{dk} \Delta(dN) = \sum_{l,\sigma} \frac{1}{\pi} \frac{\partial \delta_l(k)}{\partial k} \quad (2.160)$$

→ Total change in particle number=screening change number

$$\Delta N = \int_0^{k_F} dk \frac{d}{dk} (\Delta(dN)) = \sum_{l,\sigma} \frac{\delta_l(k_F)}{\pi} = Z \quad (2.161)$$

$$\boxed{Z = \sum_{l,\sigma} \frac{\delta_l(k_F)}{\pi}} \quad \text{Friedel sum rule} \quad (2.162)$$

