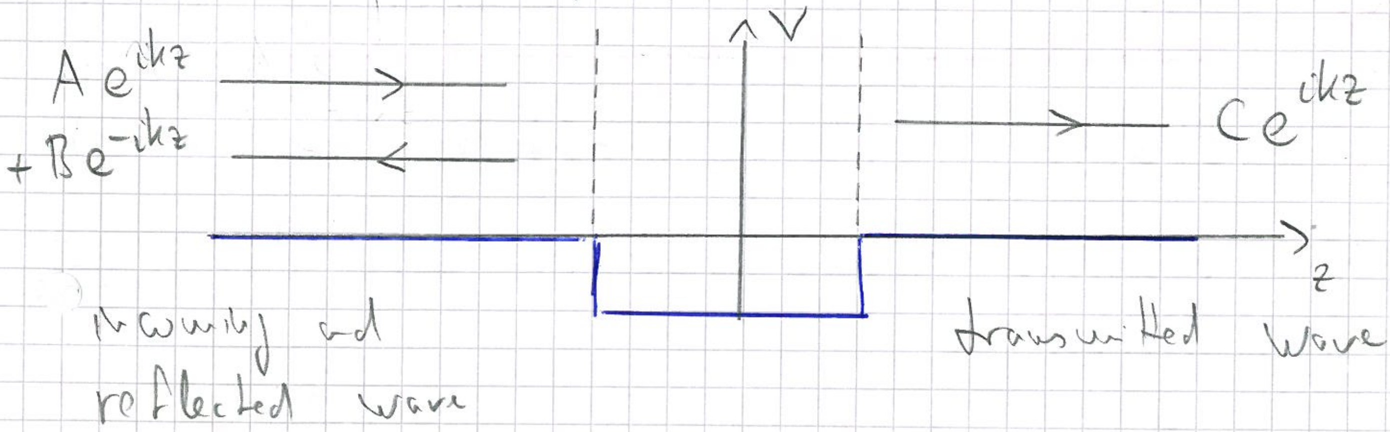
VI. Scattering theory

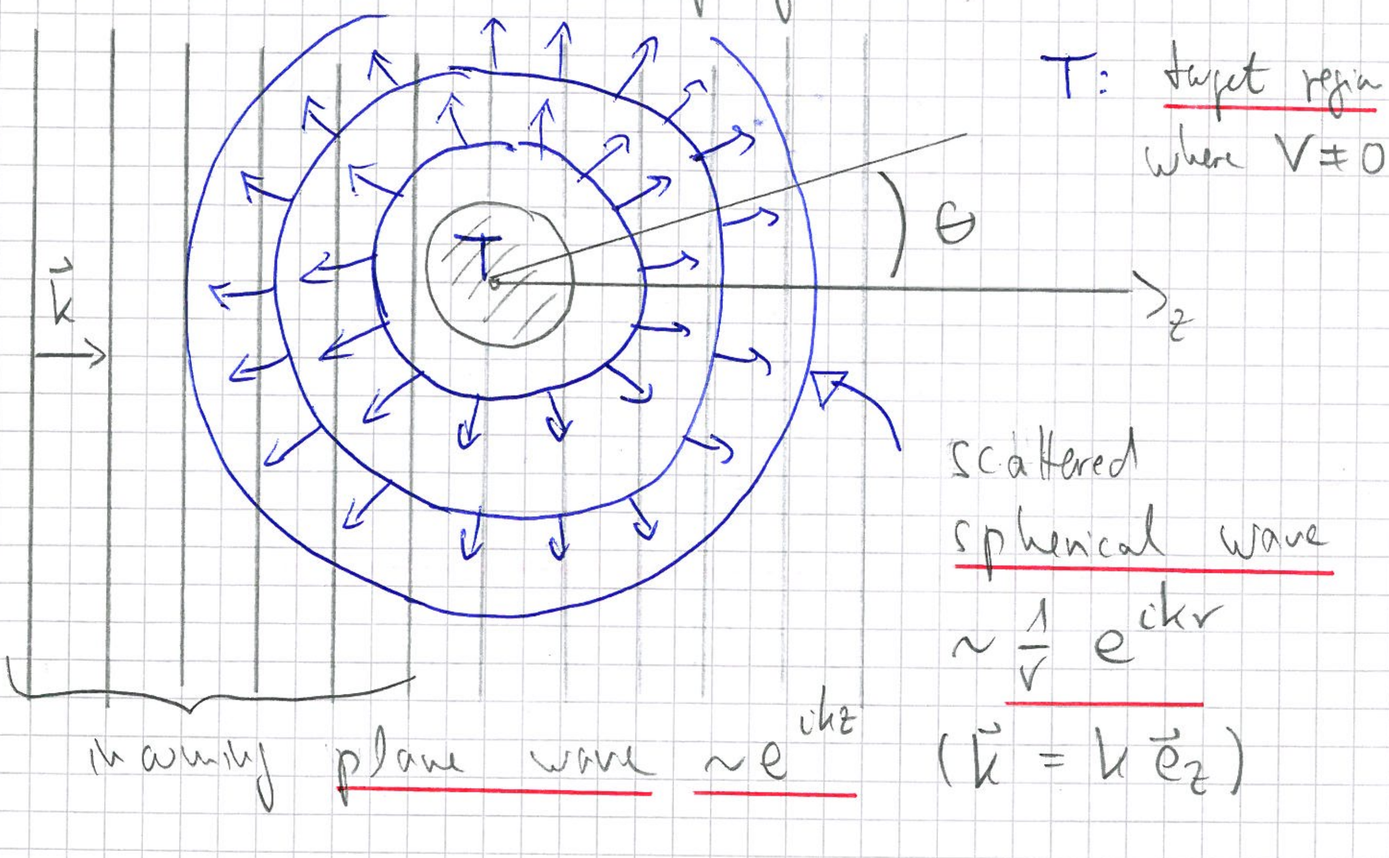
1° Stationary scattering (elastic throughout)

Reminder: Scattering in one dimension ($\rightarrow$ Problem 12.1)



Wave functions outside the potential region are solutions of the stationary Schrödinger equation with energy $E = \frac{\hbar k^2}{2m} > 0$ and momentum $\pm \hbar k$.

Three-dimensional scattering geometry:



$\Rightarrow$ outside of the target region we expect a solution of the stationary Schrödinger equation with the asymptotic form $(r \to \infty)$

$$\psi(\vec{r}) = A\left(e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\right)$$

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

The probability current associated with this wave function is

$$\vec{j} = -i\frac{\hbar}{2m}\left[\psi^* \nabla\psi - \psi\nabla\psi^*\right]$$

Specifically, the incoming current is

$$\vec{j}_{in} = |A|^2 \frac{\hbar k}{m}\vec{e}_z$$

and the radial component of the scattered current

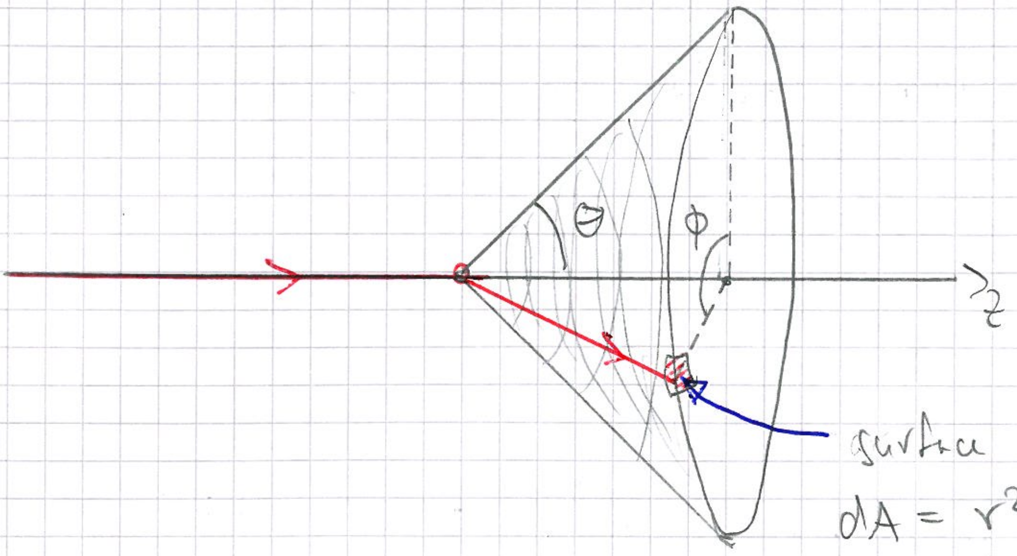
$$j_s^r = -i\frac{\hbar}{2m}\left[\psi_s^* \frac{\partial\psi_s}{\partial r} - \psi_s\frac{\partial\psi_s^*}{\partial r}\right]$$

with $\psi_s = A\, f(\theta,\phi)\frac{e^{ikr}}{r}$. This gives

$$j_s^r = |A|^2 |f(\theta,\phi)|^2 \frac{\hbar k}{m}\frac{1}{r^2}$$

The other contributions to $\vec{j}_s$ are negligible for large r.

Scattering cross section:



surface element
$$dA = r^2\, d\Omega = r^2 \sin\Theta\, d\Theta\, d\phi$$

The differential scattering cross section is the defined as follows:

$$d\sigma := \frac{\text{Number of particles through } dA \text{ per time}}{\text{incident current}}$$

$$= \frac{r^2\, d\Omega\, j^r_{scatt}}{j_{in}} = |f(\Theta,\phi)|^2\, d\Omega$$

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

Note that it follows from the definition of $f(\Theta,\phi)$ in (S) that $|f(\Theta,\phi)|^2$ has units of an area.

The total scattering cross section is the

$$\sigma_{tot} = \int d\Omega\, \frac{d\sigma}{d\Omega} = \int_0^{2\pi} d\phi \int_0^{\pi} d\Theta\, \sin\Theta\, |f(\Theta,\phi)|^2 =$$

$$= \frac{j_{tot}}{j_{in}}$$ where the integrated scattered current is

$$j_{tot} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, r^2 \sin\theta \, j^r_{scatt} =$$

$$= |A|^2 \frac{\hbar k}{m} \sigma_{tot} .$$

Problems to be addressed:

A. Find solutions of the stationary Schrödinger equation that satisfy the asymptotic boundary condition S

B. Compute $f(\theta, \phi)$ for a given potential

C. Relate the stationary approach to a more realistic (time-dependent) picture of the scattering process.

2° The scattering Green's function

Goal: Rewrite the stationary Schrödinger equation as an integral equation that automatically incorporates the boundary condition S.

The stationary Schrödinger equation reads

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi = E\psi, \quad E = \frac{\hbar^2}{2m}|\vec{k}|^2 > 0$$

$$\Rightarrow \quad \underline{\left(\nabla^2 + k^2\right)\psi = U(\vec{r})\psi} \quad \text{with } U = \frac{2m}{\hbar^2}V$$

We interpret this as a <u>Helmholtz equation</u> with a inhomogeneity $F(\vec{r}) = U(\vec{r})\psi(\vec{r})$.

<u>Def</u>: A Green's function $G_k(\vec{r},\vec{r}')$ of the Helmholtz equation satisfies

$$\underline{\left(\nabla^2 + k^2\right) G_k(\vec{r},\vec{r}') = \delta(\vec{r}-\vec{r}')}$$

Given such a Green's function, the general solution of the inhomogeneous Helmholtz eq.

$$\left(\nabla^2 + k^2\right)\psi(\vec{r}) = F(\vec{r})$$

can be constructed as

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int d^3r'\, G_k(\vec{r},\vec{r}')\, F(\vec{r}')$$

where ψ_0 is a solution of the homogeneous equation $\left(\nabla^2 + k^2\right)\psi_0 = 0$.

<u>Proof</u>: $$\left(\nabla^2 + k^2\right)\psi = \int d^3r'\, \underbrace{\left(\nabla^2 + k^2\right) G_k(\vec{r},\vec{r}')}_{=\delta(\vec{r}-\vec{r}')} F(\vec{r}')$$

$$= F(\vec{r}). \qquad \square$$

Claim: The Green's function can be chosen as (a linear combination of)

$$G_k^{(\pm)}(\vec{r},\vec{r}\,') = -\frac{1}{4\pi}\frac{e^{\pm ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|}$$

Proof: Recall that $\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta(\vec{r})$.

Moreover $\nabla^2\left(\frac{1}{r}(1-e^{\pm ikr})\right) = \frac{1}{r}\frac{d^2}{dr^2}r\left[\frac{1}{r}(1-e^{\pm ikr})\right]$

$= \frac{1}{r}k^2 e^{\pm ikr}$ because $\frac{1}{r}(1-e^{\pm ikr})$ is finite at $r=0$. Thus

$$(\nabla^2+k^2)\frac{1}{r}e^{\pm ikr} = (\nabla^2+k^2)\left(\frac{1}{r}-\frac{1-e^{\pm ikr}}{r}\right)$$

$$= -4\pi\delta(\vec{r}) - \frac{k^2}{r}e^{\pm ikr} + \frac{k^2}{r} - \frac{k^2}{r}(1-e^{\pm ikr}) =$$

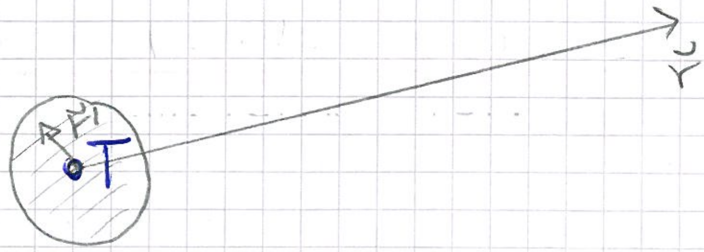
$$= -4\pi\delta(\vec{r}). \quad \square$$

We will show below that $G_k^{(+)}$ and $G_k^{(-)}$ describe outgoing and incoming spherical waves, respectively. Using $G_k^{(+)}$ the integral equation for ψ corresponding to our scattering geometry reads

$$\psi(\vec{r}) = \underbrace{e^{ikz}}_{\text{homogeneous solution}} + \int d^3r\, G_k^{(+)}(\vec{r},\vec{r}\,')\,U(\vec{r}\,')\,\psi(\vec{r}\,') =$$

$$= e^{ikz} - \frac{1}{4\pi}\int d^3r' \, \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \, U(\vec{r}')\,\psi(\vec{r}')$$

To check that the solution satisfies the boundary condition S we note that the contributions to the integral are restricted to the 'target' region where $|\vec{r}'| \ll |\vec{r}|$:



$$\Rightarrow \underline{|\vec{r}-\vec{r}'|} = \sqrt{\vec{r}^2 - 2\vec{r}\cdot\vec{r}' + \vec{r}'^2} \simeq \underline{r - \frac{\vec{r}\cdot\vec{r}'}{r}}$$

$$\Rightarrow \int d^3r' \, \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \, U(\vec{r}')\,\psi(\vec{r}') \simeq$$

$$\simeq \frac{e^{ikr}}{r} \underbrace{\int d^3r' \, e^{-ik\vec{e}_r\cdot\vec{r}'} \, U(\vec{r}')\,\psi(\vec{r}')}_{\text{depends on } \vec{e}_r = \frac{\vec{r}}{r} \text{ on } (\theta,\phi)}$$

With this we identify

$$\underline{f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int d^3r' \, e^{-i\vec{k}_{out}\cdot\vec{r}'} \, V(\vec{r}')\,\psi(\vec{r}')}$$

where $\vec{k}_{out} = k\vec{e}_r$. But note that this still depends on the unknown solution $\psi(\vec{r})$.

3° The Born approximation

If the scattering potential is weak, the solution $\psi(\vec{r})$ is dominated by the incoming plane wave and we may approximately write

$$\psi(\vec{r}) \simeq \psi_B^{(1)}(\vec{r}) = e^{ikz} - \frac{1}{4\pi}\int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}')\, e^{ikz'}$$

which defines the first Born approximation. This procedure can be iterated:

$$\psi_B^{(2)}(\vec{r}) = e^{ikz} - \frac{1}{4\pi}\int d^3r' \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}')\, \psi_B^{(1)}(\vec{r}')$$

but here we consider only the first order

The corresponding expression for the scattering amplitude reads

$$f_B(\theta,\phi) = -\frac{1}{4\pi}\int d^3r'\, e^{-i\vec{k}_{out}\cdot\vec{r}'}\, U(\vec{r}')\, e^{ikz}$$

$$= -\frac{1}{4\pi}\int d^3r'\, e^{-i(\vec{k}_{out}-\vec{k}_{in})\cdot\vec{r}'}\, U(\vec{r}')$$

where $\vec{k}_{in} = k\vec{e}_z$ is the incident wave vector.

Thus f_B is proportional to the Fourier transform of the potential evaluated at

$$\vec{K} := \vec{k}_{out} - \vec{k}_{in}$$

$\hbar\vec{K}$ is the momentum transfer.

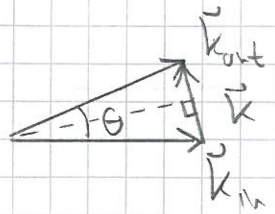
For radially symmetric potentials $V(\vec{r}) = V(r)$
the integral can be evaluated by choosing $\vec{K} = K\vec{e}_z$:

$$\int d^3r\, U(\vec{r})\, e^{-i\vec{K}\cdot\vec{r}} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \int_0^{\infty} dr\, r^2 \sin\theta\, e^{-iKr\cos\theta} \times U(r)$$

$$= 2\pi \int_0^{\infty} dr\, r^2\, U(r) \underbrace{\int_{-1}^{1} d(\cos\theta)\, e^{-iKr\cos\theta}}_{= \frac{2}{rK}\sin(Kr)}$$

$$= 4\pi K^{-1} \int_0^{\infty} dr\, r \sin(Kr)\, U(r)$$

K is related to the scattering angle θ:



$\Rightarrow$ $K = 2k \sin(\theta/2)$

$$\Rightarrow \quad f_B(\theta) = -\frac{1}{K} \int_0^{\infty} dr\, r \sin(Kr)\, U(r)$$

Example: Screened Coulomb / Yukawa potential

$$\left.\begin{aligned} V(r) &= -\frac{Ze^2}{r}\, e^{-r/\lambda} \\ \lambda &: \text{ screening length} \end{aligned}\right\}$$

$$\Rightarrow f_B(\theta) = \frac{2m}{\hbar^2}\frac{Ze^2}{K}\underbrace{\int_0^\infty dr\, \sin(Kr)\, e^{-r/\lambda}}_{= \frac{K}{K^2+\lambda^{-2}}}$$

$$= \frac{2m}{\hbar^2}\frac{Ze^2}{4k^2\sin^2(\theta/2)+\lambda^{-2}}$$

The Coulomb case is recovered by letting $\lambda \to \infty$

$$\Rightarrow f_B(\theta) = \frac{Ze^2 m}{2(\hbar k)^2 \sin^2(\theta/2)} = \frac{Ze^2 m}{2p^2\sin^2(\theta/2)}$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = |f_B(\theta)|^2 = \frac{Z^2 m^2 e^4}{4p^4\sin^4(\theta/2)}$$

This is the Rutherford cross section which is exact both in the classical and in the quantum mechanical scattering theory. It diverges as θ^{-4} for $\theta \to 0$, which implies that σ_{tot} is infinite.

Validity of the Born approximation

Replacing $\psi(\vec{r})$ by e^{ikz} in the integral equation makes a difference only in the potential region, i.e. near $\vec{r}=0$. We therefore demand that

$$\underbrace{\left|\frac{1}{4\pi}\int d^3r\,\frac{e^{ik|\vec{r}|}}{|\vec{r}|}\,U(\vec{r})\,e^{ikz}\right|}\ll\left|e^{ikz}\right|=1$$

$$=\left|\frac{1}{2}\int_{-1}^{1}d(\cos\theta)\int_0^\infty dr\,r\,U(r)\,e^{ikr}\,e^{ikr\cos\theta}\right|=$$

$$=\frac{1}{2k}\left|\int_0^\infty dr\,U(r)\left(e^{2ikr}-1\right)\right|=\underline{\frac{m}{\hbar^2k}\left|\int_0^\infty dr\,V(r)\left(e^{2ikr}-1\right)\right|}$$

$$\Downarrow$$

$$\underline{\ll 1}$$

Example: Screened Coulomb potential $-\frac{Ze^2}{r}e^{-r/\lambda}$

$$Ze^2\int_0^\infty dr\,\underbrace{\frac{1}{r}e^{-r/\lambda}}\left(e^{2ikr}-1\right)=$$

$$=\int_{1/\lambda}^{\infty}dx\,e^{-xr}$$

$$=Ze^2\int_{1/\lambda}^{\infty}dx\int_0^\infty dr\,e^{-xr}\left(e^{2ikr}-1\right)=$$

$$= Ze^2 \int_{1/\lambda}^{\infty} dx \left(\frac{1}{x - 2ik} - \frac{1}{x} \right) = -Ze^2 \ln(1 - 2ik\lambda)$$

and
$$\left. \begin{aligned} |\ln(1-2ik\lambda)|^2 &= \left(\frac{1}{2} \ln(1+4k^2\lambda^2) \right)^2 + \\ &\quad + |\mathrm{atan}(2k\lambda)|^2 \end{aligned} \right\}$$

We distinguish two cases:

(i) <u>low energies, $k\lambda << 1$:</u>

$$\ln(1+4k^2\lambda^2) \simeq 4k^2\lambda^2, \quad \mathrm{atan}(2k\lambda) \simeq 2k\lambda$$

$$\Rightarrow \frac{m}{\hbar^2 k} \cdot Ze^2 |2k\lambda| = \frac{Ze^2}{\lambda} \cdot \frac{2m\lambda^2}{\hbar^2} << 1$$

<u>Interpretation:</u> The typical potential energy at $r \simeq \lambda$ is

$$V_0 \simeq \frac{Ze^2}{\lambda}$$

and the kinetic energy of a particle confined to that scale is

$$E_{kin} \simeq \frac{\hbar^2}{2m\lambda^2}$$

$$\Rightarrow V_0 / E_{kin} << 1$$

which means that the potential is too weak to form a bound state (in three dimensions)

(ii) high energies, $k\lambda \gg 1$:

$$|\ln(1-2ik\lambda)| \simeq \frac{1}{2}\ln(4k^2\lambda^2)$$

which increases very slowly with $k\lambda$. Thus the condition reads essentially

$$\frac{m}{\hbar^2 k} \cdot Ze^2 = Z\left(\frac{e^2}{\hbar c}\right)\frac{mc}{\hbar k} = Z\alpha\frac{c}{v} \ll 1$$

where $v = p/m$ is the velocity of the incident particle and α is the fine structure constant.

Thus in this case the approximation is valid for light nuclei and high velocities.

4° Partial wave analysis

Goal: Represent the scattering problem for spherically symmetric potentials in terms of spherical harmonics.

a) Radial Schrödinger equation for free particles

Reminder: The Schrödinger Hamiltonian in spherical coordinates reads

$$H = -\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{\vec{L}^2}{2mr^2} + V(r)$$