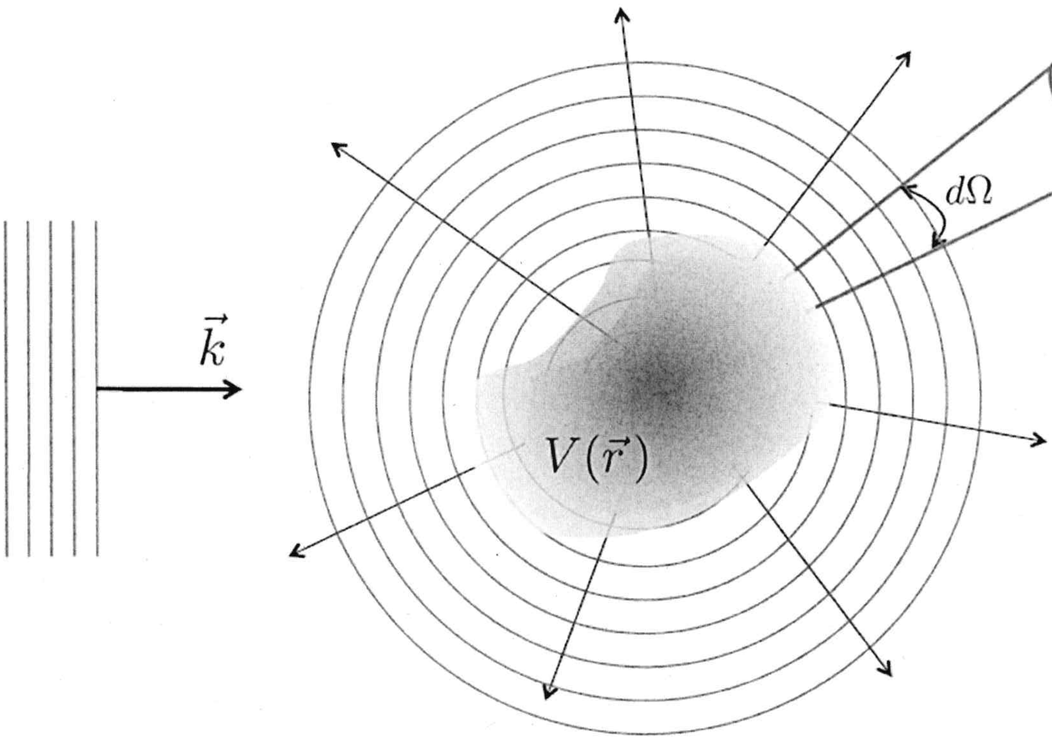
IV Scattering theory

- Scattering is of fundamental importance for making the structure of Nature „visible".
- The application of scattering has led to the discovery of the atomic nucleus (Rutherford) and scattering protons off one another is the standard tool at LHC (CERN) for searching for „new physics".
- In the following we consider the scattering of a particle of mass μ off a localised potential (i.e. the potential has a finite range, dropping off with distance $|\vec{r}|$ from the particle, sufficiently fast).
- The particle is approaching the potential from a far-away initial position.
- The particle is modelled by a wave packet, and the question we are going to ask is: What is the probability (cross section) for the particle to be scattered into the solid angle element $d\Omega$.

Scattering problem



Skript zur Vorlesung
Fortgeschrittene Quantentheorie
(Quantenmechanik II)
Prof. Werner Vogelsang
Universität Tübingen
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10.1 Scattering states and scattering cross section

- The scattering potential $U(\vec{r})$ shall be localised in the vicinity of $\vec{r} = 0$.
- The wave packet of the particle at initial time t_0 is given by

$$\psi(\vec{r}, t_0) = \int \frac{d^3\vec{k}}{(2\pi)^3} \, a(\vec{k}) \, e^{i\vec{k}\cdot\vec{r}}$$

$\uparrow$

Fourier transform of the wave packet

- The maximum of the Fourier components $a(\vec{k})$ shall be at $\vec{k}_0$, such that the particle is moving with group velocity $\frac{\hbar \vec{k}_0}{\mu}$ towards the scattering centre (potential).
- Each plane wave

$$u_k^{(0)}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}}$$

is a solution of the free, stationary Schrödinger equation

$$-\frac{\hbar^2}{2\mu} \Delta u_k^{(0)}(\vec{r}) = E_k \, u_k^{(0)}(\vec{r})$$

with the kinetic energy

$$E_k = \frac{\hbar^2 \vec{k}^2}{2\mu} = \frac{\hbar^2 k^2}{2\mu} > 0 .$$

- Our goal is to solve the time dependent Schrödinger equation

scattering potential

$$i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t} = \left[-\frac{\hbar^2}{2\mu}\Delta + U(\vec{r})\right]\psi(\vec{r},t)$$

with the boundary condition $\psi(\vec{r},t_0)$.

- In order to do this we consider at first the associated stationary problem,

$$\left[-\frac{\hbar^2}{2\mu}\Delta + V(\vec{r})\right]u_k(\vec{r}) = E_k\, u_k(\vec{r}).$$

- Here, the energy shell be fixed to $E_k = \frac{\hbar^2 k^2}{2\mu}$, which means that we are considering <u>elastic scattering</u> ($E_k > 0$, no bound states).

- The solutions $u_k(\vec{r})$ are referred to as <u>elastic scattering states</u>.

- We expect that the initial wave function can be expanded in these scattering states:

$$\psi(\vec{r},t_0) = \int \frac{d^3\vec{k}}{(2\pi)^3} A(\vec{k})\, u_k(\vec{r})$$

expansion coefficients

- The time evolved state, that we want to find is thus

$$\psi(\vec{r},t) = \int \frac{d^3\vec{k}}{(2\pi)^3} A(\vec{k})\, u_k(\vec{r})\, e^{-i\frac{E_k}{\hbar}(t-t_0)}.$$

- The „only" things left to find are the wave functions $u_k(\vec{r})$ and the expansion coefficients $A(\vec{k})$.

- In order to find the $u_k(\vec{r})$ we rewrite the stationary Schrödinger equation as

$$(\Delta + k^2)\, u_k(\vec{r}) = \underbrace{\frac{2\mu}{\hbar^2} V(\vec{r})\, u_k(\vec{r})}_{f(\vec{r})} .$$

- This looks like an inhomogeneous differential equation (it is not, because the inhomogeneity depends on $u_k(\vec{r})$).

- The next step towards solving the problem is to introduce the Green's function $G_k(\vec{r})$ which obeys

$$(\Delta + k^2)\, G_k(\vec{r}) = \delta^{(3)}(\vec{r}) .$$

- Once this is found, the stationary Schrödinger equation is „solved" by the function

$$\int d^3\vec{r}\,'\, G_k(\vec{r} - \vec{r}\,')\, f(\vec{r}\,')$$

$$\hookrightarrow (\Delta + k^2) \int d^3\vec{r}\,'\, G_k(\vec{r}\,' - \vec{r})\, f(\vec{r}\,') = \int d^3\vec{r}\,'\, \delta(\vec{r} - \vec{r}\,')\, f(\vec{r}\,') = f(\vec{r})$$

- The Green's function is found most easily in Fourier space:

$$G_k(\vec{r}) = \int \frac{d^3\vec{q}}{(2\pi)^3}\, \tilde{G}_k(\vec{q})\, e^{i\vec{q}\cdot\vec{r}} .$$

- Then $$(\Delta^2+k^2)\,G_k(\vec r) = \int \frac{d^3\vec q}{(2\pi)^3}\,\tilde G_k(\vec q)\,(\Delta+k^2)\,e^{i\vec q\cdot\vec r}$$
$$= \int \frac{d^3\vec q}{(2\pi)^3}\,\tilde G_k(\vec q)\,(-\vec q^{\,2}+k^2)\,e^{i\vec q\cdot\vec r}$$
$$\overset{!}{=} \delta^3(\vec r) = \int d^3\vec q\; 1\; e^{i\vec q\cdot\vec r}$$

$\hookrightarrow$ $$\tilde G_k(\vec q) = \frac{1}{k^2-\vec q^{\,2}} = \frac{1}{k^2-q^2}$$

- In order to obtain the Green's function in real space, we need to calculate the Fourier transform

$$G_k(\vec r) = \int \frac{d^3\vec q}{(2\pi)^3}\,\frac{e^{i\vec q\cdot\vec r}}{k^2-q^2} = \frac{1}{(2\pi)^3}\int_0^\infty dq\,q^2 \int_{-1}^{1} d\cos\theta \int_0^{2\pi} d\varphi\; \frac{e^{iqr\cos\theta}}{k^2-q^2}$$

$$= \frac{2\pi}{(2\pi)^3}\int_0^\infty dq\,\frac{q^2}{k^2-q^2}\int_{-1}^{1} d\cos\theta\; e^{iqr\cos\theta}$$

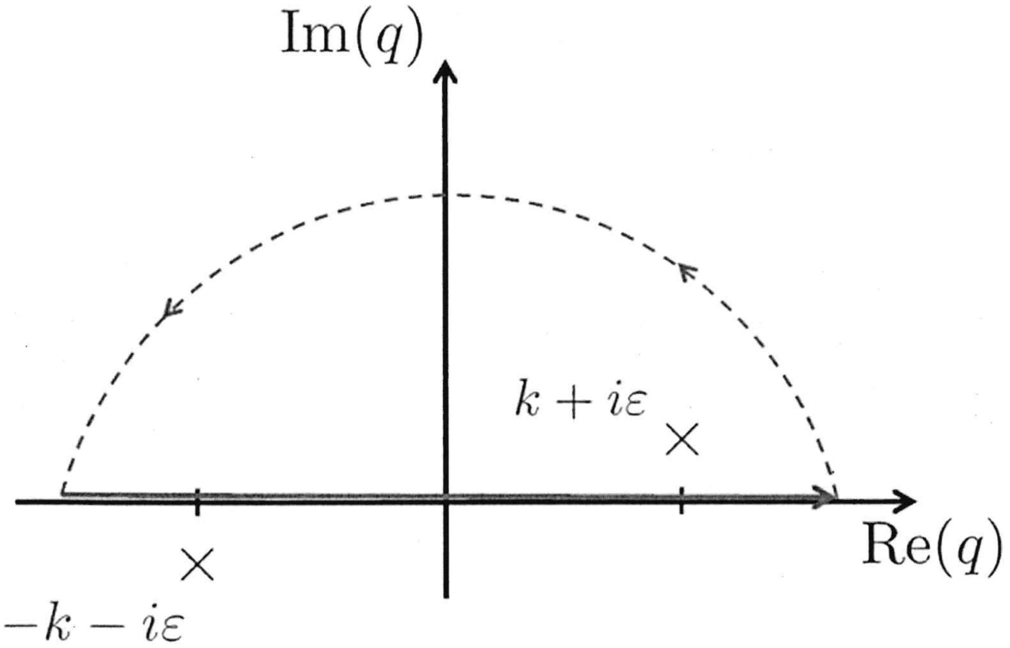
$$= \frac{1}{(2\pi)^2}\int_0^\infty dq\,\frac{q^2}{k^2-q^2}\,\frac{1}{iqr}\left(e^{iqr}-e^{-iqr}\right)$$

$$= -\frac{1}{(2\pi)^2}\,\frac{1}{2ir}\int_{-\infty}^{\infty} dq\left(\frac{1}{q-k}+\frac{1}{q+k}\right)e^{iqr}.$$

- The integrals diverge, which means that the inverse of Δ^2+k^2 is not uniquely defined.
- To nevertheless solve the integration, we introduce an imaginary part to the k

$\hookrightarrow$ $k \to k+i\varepsilon \quad (\varepsilon>0)$.

Integration contour for Green's function



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- We can now use the residue theorem to calculate the integral.
- Closing the contour in the upper half-plane, since here the factor e^{iqr} is suppressing the contribution of the contour, yields

$$\int_{-\infty}^{\infty} dq \left(\frac{1}{q-(k+i\varepsilon)} + \frac{1}{q+(k+i\varepsilon)} \right) e^{iqr} = 2\pi i \, \mathrm{Res} \left(\frac{e^{iqr}}{q-(k+i\varepsilon)} \right)_{q=k+i\varepsilon}$$

$$= 2\pi i \, e^{i(k+i\varepsilon)r} \xrightarrow{\varepsilon \to 0} 2\pi i \, e^{ikr}$$

- Hence, the Green's function is

$$G_k(\vec{r}) = -\frac{1}{4\pi} \frac{e^{ikr}}{r},$$

which represents a spherical wave.
- With its help the solution of the stationary Schrödinger equation is given by

$$u_k(\vec{r}) = -\frac{1}{4\pi} \int d^3\vec{r}\,' \, \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} f(\vec{r}\,').$$

- This expression describes a wave that is <u>outgoing</u> with respect to the scattering centre.
- This is seen by the fact that the combination with the phase factor of the free time evolution yields $e^{i(k|\vec{r}-\vec{r}\,'| - \frac{E_k}{\hbar}(t-t_0))}$, and therefore shells of constant phase have a radius that grows with time

- For that reason one refers also to the calculated Green's function as <u>retarded Green's function</u>.
- Note, that choosing $\varepsilon < 0$ would have led to the advanced Green's function, $G_k^-(\vec{r}) = -\frac{1}{4\pi} \frac{e^{-ikr}}{|\vec{r}-\vec{r}\,'|}$ which we do not consider for physical reasons.
- The solution for $u_k(\vec{r})$ that we constructed is still incomplete, which is seen by the fact that it vanishes for $V(\vec{r}) = f(\vec{r}) = 0$, and therefore it is not compatible with the imposed boundary condition
- This is cured by adding the incoming plane wave $u_k^{(0)}(\vec{r})$, which solves the equation $(\Delta + k^2) u_k^{(0)}(\vec{r}) = 0$ and thus does not change the fact that $u_k(\vec{r})$ must solve the inhomogeneous problem.
- With this modification we obtain the so-called <u>Lipmann-Schwinger equation</u>:

$$u_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \int d^3 r' \, \frac{e^{ik|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} \frac{2\mu}{\hbar} V(\vec{r}\,') \, u_k(\vec{r}\,').$$

- This equation can be solved by iteration.
- It shows that the solution of the scattering problem is composed of an incoming plane wave and a scattered wave, which is a superposition of spherical waves.

- In the next step we simplify the integrand, assuming that the detector, with which we probe the scattering solution is far away from the scattering centre.
- We use

$$|\vec{r}-\vec{r}\,'| = \sqrt{r^2 - 2\vec{r}\cdot\vec{r}\,' + r'^2} = r\sqrt{1 - \frac{2\vec{r}\cdot\vec{r}\,'}{r^2} + \left(\frac{r'}{r}\right)^2}$$

$$\approx r\left(1 - \frac{\vec{r}\cdot\vec{r}\,'}{r^2}\right) = r - \vec{e}_r\cdot\vec{r}\,'$$

radial unit vector

and make the approximations

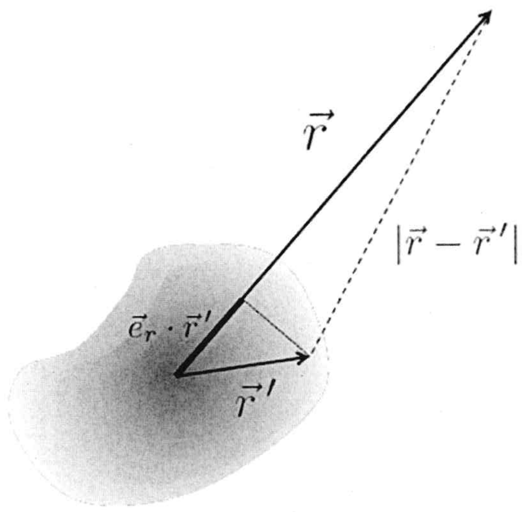
$$\underbrace{\frac{1}{|\vec{r}-\vec{r}\,'|} \approx \frac{1}{r}}_{\text{first order is sufficient}} \quad \text{and} \quad e^{ik|\vec{r}-\vec{r}\,'|} \approx e^{ikr}\, e^{-ik\vec{e}_r\cdot\vec{r}\,'}$$

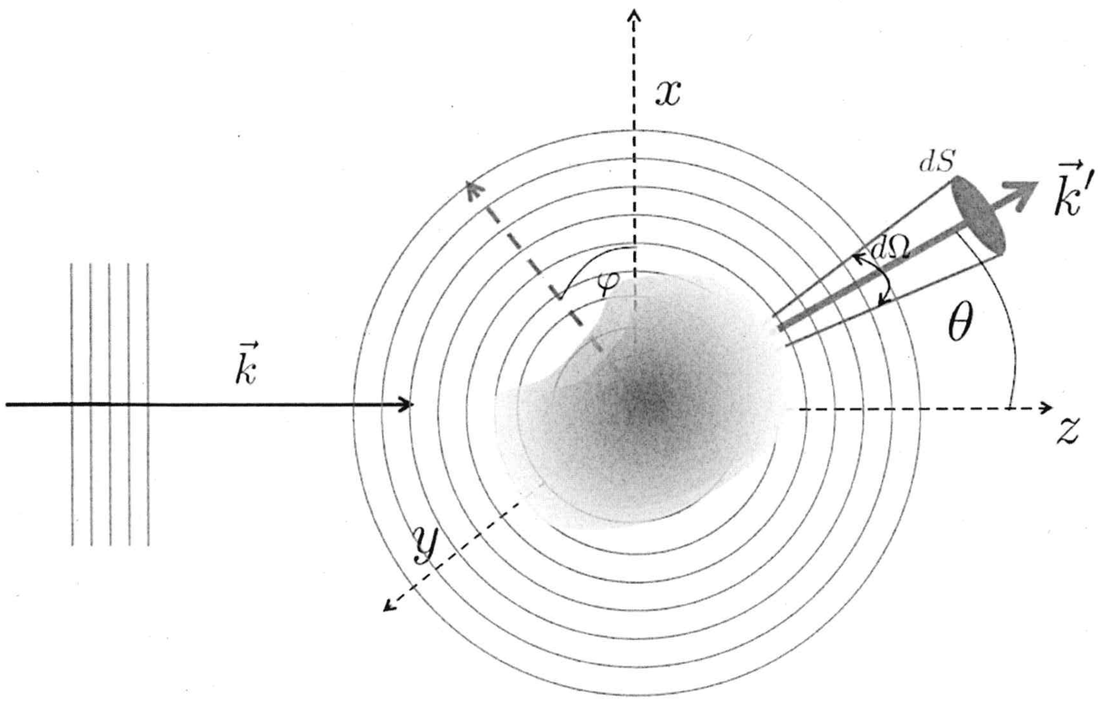
- This yields

$$u_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi}\frac{e^{ikr}}{r}\int d^3\vec{r}\,'\, e^{-ik\vec{e}_r\cdot\vec{r}\,'}\frac{2\mu}{\hbar}V(\vec{r}\,')\,u_k(\vec{r}\,')$$

$$\equiv e^{i\vec{k}\cdot\vec{r}} + f_k(\theta,\varphi)\,\frac{e^{ikr}}{r}.$$

Geometry of the scattering problem





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- In the last step we have introduced the so-called <u>scattering amplitude</u>

$$f_k(\theta,\varphi) = -\frac{1}{4\pi}\int d^3r' \, e^{-ik\vec{e}_r \cdot \vec{r}'} \frac{2\mu}{\hbar^2} V(\vec{r}')\, u_k(\vec{r}') .$$

- Note, that $f_k(\theta,\varphi)$ only depends on $\vec{e}_r$ and has the unit 'length'.

- The position vector $\vec{r}$ is the vector at which one observes the scattering solution with the detector.

- Moreover, the vector $\vec{k}' = k\vec{e}_r$ points into the direction of $\vec{r}$.

- This means that $f_k(\theta,\varphi)$ is the probability amplitude for the scattering of the incoming wave into the direction $\vec{k}'$.

- It is also the probability amplitude for detecting the scattered particle at position $\vec{r}$.

- The fact that $|\vec{k}'| = |\vec{k}|$ is once again a manifestation of elastic scattering.

- It is common to align the z-axis of the coordinate system with the wave vector of the incoming wave: $\vec{k} = k\vec{e}_z$.

- We now imagine a scenario in which a particle beam (the particles do not interact with one another) scatters off the scattering centre.

- We can then define the scattering cross section $d\sigma$ for the scattering of a particle into the solid angle element $d\Omega$:

$$d\sigma = \frac{\#\text{ particles per time scattered into } d\Omega}{\text{incoming particle flux}}$$

$$= \frac{|\vec{j}^{\,out}(\vec{k}')|\, dS}{|\vec{j}^{\,in}(\vec{k})|} = \frac{|\vec{j}^{\,out}(\vec{k}')|\, \overbrace{r^2\, d\Omega}^{dS \text{ .. surface element}}}{|\vec{j}^{\,in}(\vec{k})|}$$

- The incoming and outgoing currents we calculate using $u_k^{(0)} = e^{i\vec{k}\cdot\vec{r}}$ and

$$\vec{j}^{\,in} = \frac{\hbar}{2\mu i}\left[(u_k^{(0)})^* \nabla u_k^{(0)} - (\nabla u_k^{(0)})^* u_k^{(0)}\right] = \frac{\hbar\vec{k}}{\mu}$$

as well as $u_k^{out} = f(\theta,\varphi)\,\frac{e^{ikr}}{r}$ and

$$\vec{j}^{\,out} = \frac{\hbar}{2\mu i}\left[(u_k^{out})^* \nabla u_k^{out} - (\nabla u_k^{out})^* u_k^{out}\right]$$

$$= \frac{\hbar k\,\vec{e}_r}{\mu}\,\frac{|f_k(\theta,\varphi)|^2}{r^2} = \frac{\hbar\vec{k}'}{\mu}\,\frac{|f_k(\theta,\varphi)|^2}{r^2}$$

- Hence, we find

$$d\sigma = \underbrace{\frac{|\vec{k}'|}{|\vec{k}|}}_{=1} \frac{|f_k(\theta,\varphi)|^2}{r^2} r^2 d\Omega ,$$

and for the <u>differential scattering cross section</u> we obtain

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

which has the unit $(\text{length})^2$.

- The total scattering cross section then follows from integration:

$$\sigma = \int d\Omega \, \frac{d\sigma}{d\Omega} = \int d\Omega \, |f_k(\theta,\varphi)|^2 .$$

- From these expressions it becomes apparent that all relevant information on the scattering problem is contained in the scattering amplitude $f_k(\theta,\varphi)$.

- We will now start to solve the Lippmann-Schwinger equation, in order to calculate an (approximate) expression for the scattering amplitude

- To this end we insert the Lippmann-Schwinger equation into itself:

$$u_k(\vec r) = e^{i\vec k\cdot\vec r} + \int d^3\vec r\,' \, G_k(\vec r-\vec r\,') \frac{2\mu}{\hbar^2} V(\vec r\,') u_k(\vec r\,')$$

$$= e^{i\vec k\cdot\vec r} + \int d^3\vec r\,' \, G_k(\vec r-\vec r\,') \frac{2\mu}{\hbar^2} V(\vec r\,') e^{i\vec k\cdot\vec r\,'}$$

$$+ \int d^3\vec r\,' G_k(\vec r-\vec r\,') \frac{2\mu}{\hbar} V(\vec r\,') \int d^3\vec r\,'' G_k(\vec r\,'-\vec r\,'') \frac{2\mu}{\hbar} V(\vec r\,'') u_k(\vec r\,'')$$

- Such iteration step can of course be repeated indefinitely, yielding the <u>Born series</u>

$$u_k(\vec r) = \sum_{n=0}^{\infty} u_k^{(n)}(\vec r)$$

with $u_k^{(0)}(\vec r) = e^{i\vec k\cdot\vec r}$

and $u_k^{(n)}(\vec r) = \int d^3\vec r\,' \, G(\vec r-\vec r\,') \frac{2\mu}{\hbar^2} V(\vec r\,') u_k^{(n-1)}(\vec r\,')$.

- Truncation of this series at the n-term corresponds to the Born approximation of order n
- In the following we consider the Born approximation of order 1 (first Born approximation) more closely:

$$u_k(\vec r) = e^{i\vec k\cdot\vec r} - \frac{1}{4\pi} \int d^3\vec r\,' \frac{e^{ik|\vec r-\vec r\,'|}}{|\vec r-\vec r\,'|} \frac{2\mu}{\hbar^2} V(\vec r\,') e^{i\vec k\cdot\vec r\,'}$$

$|\vec r|$ is much larger than interaction range

$$\approx e^{i\vec k\cdot\vec r} - \frac{1}{4\pi}\frac{e^{ikr}}{r} \int d^3\vec r\,' e^{-ik\vec e_r\cdot\vec r\,' + i\vec k\cdot\vec r\,'} V(\vec r\,')$$

(- This first Born approximation usually works well when the interaction is weak or the energy of the incident particle is high.)

- Comparing this result with the general scattering solution (p 144) yields the scattering amplitude:

$$f_k^B(\theta,\varphi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int d^3\vec{r}\,' \, e^{-ik\vec{e}_r\cdot\vec{r}\,' + i\vec{k}\cdot\vec{r}\,'} \, V(\vec{r}\,')$$

- Writing $-ik\vec{e}_r\cdot\vec{r}\,' + i\vec{k}\cdot\vec{r}\,' = i(\vec{k}-\vec{k}\,')\cdot\vec{r}\,' = i\underset{\uparrow}{\vec{q}}\cdot\vec{r}\,'$

yields the more compact expression $\qquad$ momentum transfer

$$f_k^B(\theta,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int d^3\vec{r}\,' e^{i\vec{q}\cdot\vec{r}\,'}V(\vec{r}\,') .$$

- Hence the scattering amplitude within the first Born approximation is the Fourier transform of the interaction potential with respect to the momentum transfer, and the differential cross-section becomes

$$\frac{d\sigma^B}{d\Omega} = |f_k^B(\theta,\varphi)|^2 = \frac{\mu^2}{4\pi^2\hbar^4}\left|\int d^3\vec{r}\, e^{i\vec{q}\cdot\vec{r}}\, V(\vec{r})\right|^2 .$$

- An important case is the scattering off a spherically symmetric potential, $V(\vec{r}) = V(r)$, for which one obtains

$$f_k^B(\theta) = -\frac{\mu}{2\pi\hbar^2}\int_0^\infty dr\, r^2 V(r)\int_0^{2\pi} d\varphi \int_{-1}^{1} d\cos\theta\, e^{iqr\cos\theta}$$

$$= -\frac{\mu}{\hbar^2}\int_0^\infty dr\, r^2 V(r)\,\frac{1}{iqr}\left(e^{iqr} - e^{-iqr}\right)$$

$$= -\frac{2\mu}{q\hbar^2}\int_0^\infty dr\, r\, V(r)\, \sin(qr)$$

- The relation between the scattering angle θ and the momentum transfer q is established via the relation

$$q = |\vec{k} - \vec{k}'| = \sqrt{k^2 + k'^2 - 2\vec{k}\cdot\vec{k}'} = k\sqrt{2(1-\cos\theta)} = 2k\sin\left(\frac{\theta}{2}\right).$$

- Example: Yukawa-potential, which serves as a model potential for describing nuclear forces.

$$V(r) = -\underbrace{g^2}_{\text{interaction strength}} \frac{e^{-\overbrace{a}^{\text{inverse interaction range}} r}}{r}$$

$\hookrightarrow$ $$f_k^B(\theta) = \frac{2\mu g^2}{q\hbar^2}\int_0^\infty dr\, e^{-ar}\sin(qr)$$

$$= \frac{2\mu g^2}{\hbar^2}\frac{1}{a^2+q^2} = \frac{2\mu g^2}{\hbar^2}\frac{1}{a^2+4k^2\sin^2\frac{\theta}{2}}$$

$\hookrightarrow$ $$\frac{d\sigma^B}{d\Omega} = \frac{4\mu^2 g^4}{\hbar^4}\frac{1}{\left[a^2+4k^2\sin^2\frac{\theta}{2}\right]^2}.$$

- Let us now return to the description of the <u>scattering process in terms of wave packets</u>, with which we started the discussions of this chapter.

- We write the wave packet of the incoming particle as

$$\psi^{in}(\vec{r}, t_0) = \int \frac{d^3k}{(2\pi)^3}\, a(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}.$$

- The coefficients $a(\vec{k})$ shall be peaked around a certain $\vec{k}_0$, e.g.

$$a(\vec{k}) \sim e^{-g(\vec{k}-\vec{k}_0)^2}$$

constant controls width of wave packet ($g>0$)

for a Gaussian wave packet.

- We also assume that the wave packet is well localised in real space, i.e., the constant g cannot be too large.

- We now look for an expansion of the wave packet in terms of the scattering solutions $u_k(\vec{r})$:

$$\psi^{in}(\vec{r}, t_0) = \int \frac{d^3k}{(2\pi)^3}\, A(\vec{k})\, u_k(\vec{r}).$$

- Rewriting the Lippmann-Schwinger equation yields

$$e^{i\vec{k}\cdot\vec{r}} = u_k(\vec{r}) + \frac{1}{4\pi}\int d^3r' \,\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\,\frac{2\mu}{\hbar^2} V(\vec{r}')\, u_k(\vec{r}').$$

- Inserting this expression into the expansion of $\psi^{in}(\vec r, t_0)$ in terms of plane waves leads to

$$\psi^{in}(\vec r, t_0) = \underbrace{\int \frac{d^3\vec k}{(2\pi)^3}\, a(\vec k)\Big[u_k(\vec r)}_{\text{has the form we are looking for}} + \underbrace{\frac{1}{4\pi}\int d^3\vec r\,' \frac{e^{ik|\vec r-\vec r\,'|}}{|\vec r-\vec r\,'|}\frac{2\mu}{\hbar^2}V(\vec r\,')u_k(\vec r\,')\Big]}_{\text{term can be neglected, when integrating over } \vec k}.$$

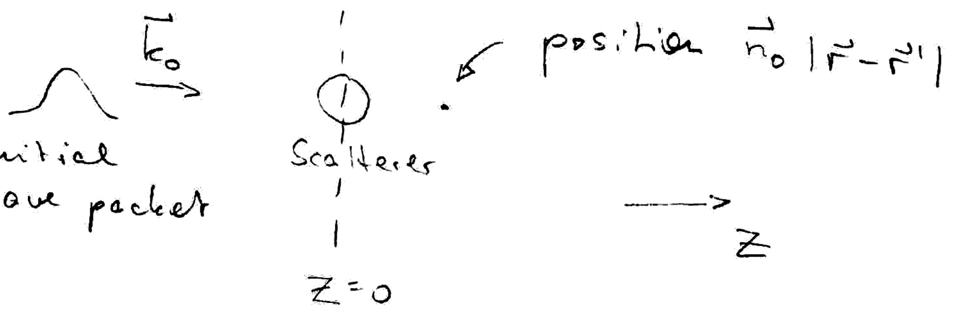
- We consider only the $\vec k$-dependent parts of the second term:

$$\int \frac{d^3\vec k}{(2\pi)^3} \underbrace{a(\vec k)}_{\text{peaked at } \vec k=\vec k_0} \underbrace{e^{ik|\vec r-\vec r\,'|}}_{\approx e^{i\left(\vec k\cdot\frac{\vec k_0}{|\vec k_0|}\right)|\vec r-\vec r\,'|}} \underbrace{u_k(\vec r\,')}_{\approx u_{k_0}(\vec r\,')} \approx u_{k_0}(\vec r)\underbrace{\int \frac{d^3\vec k}{(2\pi)^3}\, a(\vec k)\, e^{i\vec k\cdot\vec n_0|\vec r-\vec r\,'|}}_{\psi^{in}(\vec n_0|\vec r-\vec r\,'|,\, t_0)}$$

$\vec n_0 = \frac{\vec k_0}{|\vec k_0|}$

$\left(\vec k\cdot\frac{\vec k_0}{|\vec k_0|}\right)$: projection of $\vec k$ onto direction of $\vec k_0$

- The second term thus depends on the value of the initial wave packet at position $\vec n_0|\vec r-\vec r\,'|$, which is a point at the right of the scattering centre:



- However, here the wave packet is zero and thus the second term vanishes

- Therefore,

$$\psi^{in}(\vec{r},t_0) = \int \frac{d^3\vec{k}}{(2\pi)^3}\, a(\vec{k})\, u_k(\vec{r})$$

$\hookrightarrow$ $A(\vec{k}) = a(\vec{k})$, i.e. the expansion coefficients are the same as for plane waves.

- The time evolved state then becomes

$$\psi(\vec{r},t) = \int \frac{d^3\vec{k}}{(2\pi)^3}\, a(\vec{k})\, u_k(\vec{r})\, e^{-i\frac{E_k}{\hbar}(t-t_0)} \qquad E_k = \frac{\hbar^2 k^2}{2\mu}$$

$$= \int \frac{d^3\vec{k}}{(2\pi)^3}\, a(\vec{k})\, e^{i\vec{k}\cdot\vec{r}}\, e^{-i\frac{E_k}{\hbar}(t-t_0)} + \int \frac{d^3\vec{k}}{(2\pi)^3}\, a(\vec{k})\, f_k(\theta,\varphi)\, \frac{e^{ikr}}{r}\, e^{-i\frac{E_k}{\hbar}(t-t_0)}$$

$$\approx \int \frac{d^3\vec{k}}{(2\pi)^3}\, a(\vec{k})\, e^{i(\vec{k}\cdot\vec{r}-\frac{E_k}{\hbar}(t-t_0))} + \frac{f_{k_0}(\theta,\varphi)}{r} \int \frac{d^3\vec{k}}{(2\pi)^3}\, a(\vec{k})\, e^{i[(\vec{n}_0\cdot\vec{k})r - \frac{E_k}{\hbar}(t-t_0)]}$$

exploiting that $a(\vec{k})$ is peaked around $\vec{k}_0$

$$= \psi^{in}(\vec{r},t) + \frac{f_{k_0}(\theta,\varphi)}{r}\, \underbrace{\psi^{in}(\vec{n}_0 r, t)}_{\text{incoming wave packet evaluated at new position}}$$

- To interpret this expression it is instructive to study a Gaussian initial wave packet

incoming wave packet: $\psi^{in}(\vec{r},t) \sim e^{-g'(\vec{r}-\vec{v}_g t)^2}$

group velocity $\vec{v}_g = \frac{\hbar \vec{k}_0}{\mu} = \frac{\hbar k_0}{\mu}\vec{n}_0$

Wave packet moves into the direction of $\vec{v}_g$ $\quad \vec{n}_0 \parallel \vec{v}_g$

scattered wave packet: $\psi^{in}(r\vec{n}_0,t) \sim e^{-g'(\vec{n}_0 r-\vec{v}_g t)^2} = e^{-g'(r-|\vec{v}_g|t)^2}$

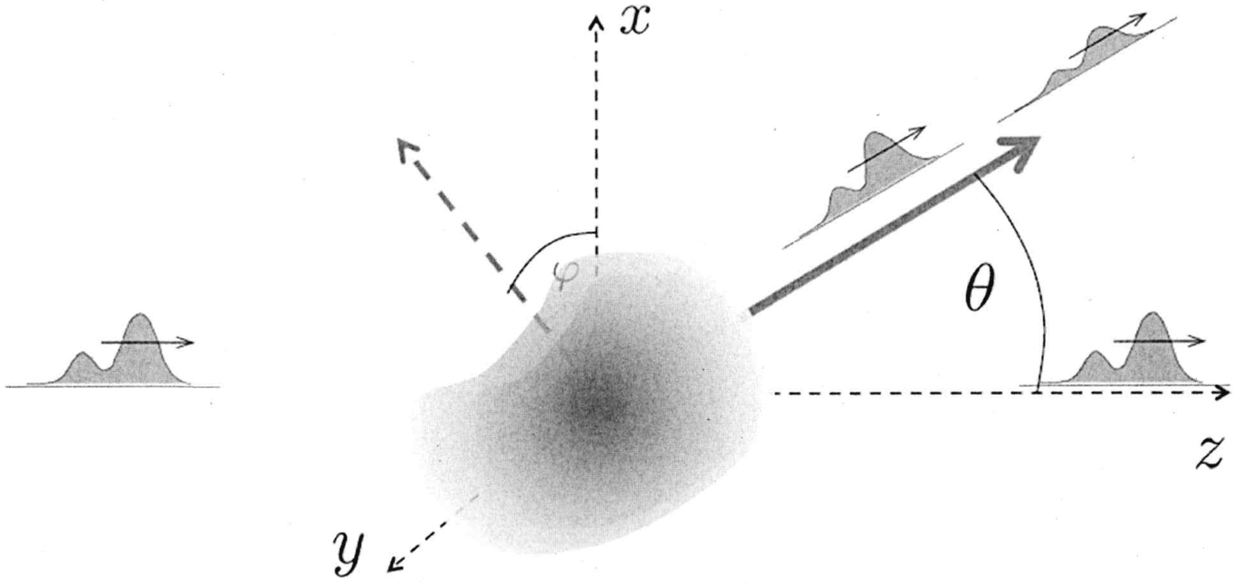
Wave packet is moving radially outwards, i.e. the wave front has the shape of a sphere

- In the following we study the probability current more closely, which will lead us to the so-called <u>optical theorem</u>

- The probability density $\rho = |\psi|^2$ and the current $\vec{j} = \frac{\hbar}{2\mu i}(\psi^* \nabla\psi - \psi\nabla\psi^*)$ of a state ψ are connected by the continuity equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\vec{j} = 0 .$$

Scattering process with wave packets



Skript zur Vorlesung
Fortgeschrittene Quantentheorie
(Quantenmechanik II)
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- In a stationary situation one has $\frac{\partial \varrho}{\partial t} = 0$ and therefore $\nabla \cdot \vec{j} = 0$.

- Integration of this expression over the volume of a large sphere, which encloses the scattering centre yields

$$0 = \int_{\text{sphere}} d^3\vec{r}\, \nabla \cdot \vec{j} = \int_{\text{surface}} d\vec{A} \cdot \vec{j} = r^2 \int_{\text{surface}} d\Omega\, \underbrace{\vec{j} \cdot \vec{e}_r}_{} \equiv r^2 \int_{\text{surface}} d\Omega\, \underbrace{j_r}_{}$$

radial current component

- We calculate in the following the radial component, j_r, of the current for the scattering state

$$u_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + f_k(\theta, \varphi) \frac{e^{ikr}}{r}.$$

$$j_r = \frac{\hbar}{2\mu i}\left(u_k^* \frac{\partial}{\partial r} u_k - u_k \frac{\partial}{\partial r} u_k^*\right) = \frac{\hbar}{\mu} \operatorname{Im}\left[u_k^* \frac{\partial}{\partial r} u_k\right]$$

$$\overset{\vec{k} = k\vec{e}_z}{=} \frac{\hbar}{\mu} \operatorname{Im}\left[\left(e^{-ikr\cos\theta} + f_k^* \frac{e^{-ikr}}{r}\right) \frac{\partial}{\partial r}\left(e^{ikr\cos\theta} + f_k \frac{e^{ikr}}{r}\right)\right]$$

$$\overset{\text{large } r}{\approx} \frac{\hbar}{\mu} \operatorname{Im}\left[\left(e^{-ikr\cos\theta} + f_k^* \frac{e^{-ikr}}{r}\right)\left(ik\cos\theta\, e^{ikr\cos\theta} + ik f_k \frac{e^{ikr}}{r} + \underbrace{\mathcal{O}\left(\tfrac{1}{r^2}\right)}_{\text{neglected}}\right)\right]$$

$$= \underbrace{\frac{\hbar}{\mu} k\cos\theta}_{\equiv\, j_r^{in}} + \underbrace{\frac{\hbar k}{\mu} \frac{|f_k|^2}{r^2}}_{j_r^{out}} + \underbrace{\frac{\hbar k}{\mu r} \operatorname{Im}\left[i\left(f_k^* e^{-ikr(1-\cos\theta)} \cos\theta + f_k e^{ikr(1-\cos\theta)}\right)\right]}_{j_r^{int}}$$

j_r^{in}: incoming; j_r^{out}: outgoing; j_r^{int}: interference current

- Integrating the current of the incoming wave yields $\int d\Omega\, j_r^{in} = 0$.

- For the current of the outgoing spherical wave one obtains the integral

$$\int d\Omega\, j_r^{out} = \frac{\hbar k}{\mu} \int d\Omega \frac{|f_k(\theta,\varphi)|^2}{r^2} = \frac{\hbar k}{\mu r^2}\, \sigma$$

total scattering cross section

- The current of the interfering incoming and outgoing wave yields the integral

$$\int d\Omega\, j_r^{int} = \int_0^{2\pi} d\varphi \int_{-1}^{1} d\cos\theta\, \frac{\hbar k}{\mu r} \operatorname{Im}\left[i \left(f_k^*(\theta,\varphi)\, e^{-ikr(1-\cos\theta)} \cos\theta + f_k(\theta,\varphi)\, e^{ikr(1-\cos\theta)} \right) \right]$$

- For large r-values the exponential functions are rapidly oscillating, except when $\theta = 0$ $(\cos\theta = 1)$.
- Choosing r sufficiently large, the only contribution to the integral comes therefore from angles around $\theta = 0$.
- Moreover, at $\theta = 0$ there is no dependence of the scattering amplitude f_k on φ ($f_k(0,\varphi) \to f_k(0)$)
- We can therefore approximate:

$$\int d\Omega\, j_r^{int} \approx \frac{2\pi\hbar k}{\mu r} \int_{-1}^{1} d\cos\theta\, \operatorname{Im}\left[i \left(f_k^*(0)\, e^{-ikr(1-\cos\theta)} + f_k(0)\, e^{ikr(1-\cos\theta)} \right) \right]$$

$$\approx \frac{2\pi\hbar k}{\mu r} \operatorname{Im}\left[\frac{f_k^*(0)}{kr} - \frac{f_k(0)}{kr} \right] = -\frac{4\pi\hbar}{\mu r^2} \operatorname{Im}\left[f_k(0) \right].$$

- Note, that after the integration step we omitted terms of the form $e^{\pm 2ikr}$ which also rapidly oscillate for large r.
- Putting everything together yields

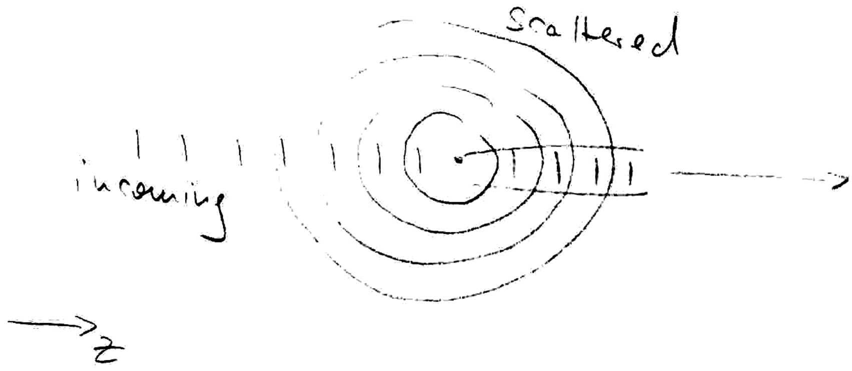
$$0 = \underbrace{0}_{j_r^{in}} + \underbrace{\frac{\hbar k}{\mu r^2}\sigma}_{j_r^{out}} - \underbrace{\frac{4\pi\hbar}{\mu r^2}\,\mathrm{Im}\left[f_k(0)\right]}_{j_r^{int}}$$

$$\hookrightarrow \quad \sigma = \frac{4\pi}{k}\,\mathrm{Im}\left[f_k(\theta=0)\right].$$

- This relationship between the total scattering cross section and the imaginary part of the scattering amplitude in forward direction is the so-called <u>optical theorem</u>.
- It has the following interpretation / consequences:

i) The current of the outgoing (scattered) wave and the current related to the interference of the scattered and incoming wave cancel.

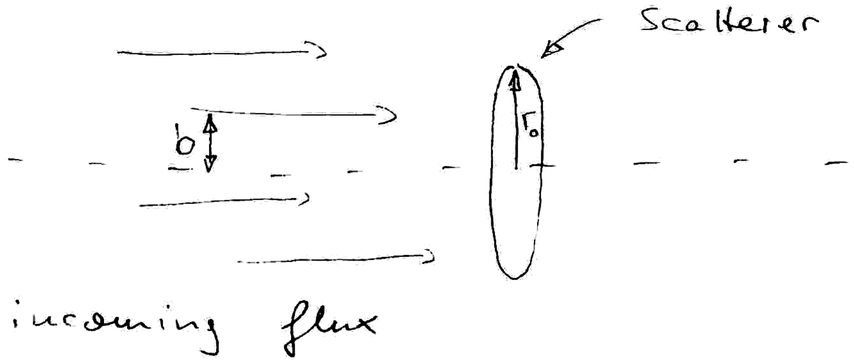
ii) The scattering amplitude cannot be real everywhere.



interference reduces current in forward direction, so that incoming and outgoing currents are equal

IV. 2 Partial wave decomposition

- We will now focus more closely on the case of a spherically symmetric scatterer
- In this case we have conservation of angular momentum.
- It is then convenient to decompose the incident wave packet into its angular momentum components, since each one of these scatters independently.
- This idea is called <u>partial wave decomposition</u>, and to see that this can be indeed advantageous, lets consider this „classical" setting.



- The angular momentum of an incoming particle is $L = b \cdot p$ ← momentum
  ↑ distance from the axis (impact parameter)
- According to the sketch only particles with $b \leq r_0$ are hitting the disk of the scatteror.
- Quantum mechanically $L \approx \hbar l$.
  ↑ angular momentum quantum number

- Thus, for particles that undergo scattering off the scattering disk we find

$$L \approx \hbar l \leq r_0 p = r_0 \hbar k$$

$$\hookrightarrow \quad l \leq k r_0 .$$

- One would thus expect that the quantity kr_0 determines how many partial waves (angular momentum components) have to be considered in the scattering process.

- To study this problem rigorously, we consider the Hamiltonian for a particle in a spherically symmetric potential $V(r)$:

$$H = -\frac{\hbar^2}{2\mu}\Delta + U(r) = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\vec{L}^2}{2\mu r^2} + U(r),$$

with $\vec{L}^2$ being the squared angular momentum operator.

- The operators H, $\vec{L}^2$ and L_z commute and the eigenfunctions of H can be constructed such that they are eigenfunctions to all of these operators.

- They have the form

$$\Psi(r,\theta,\varphi) = \underbrace{R(r)}_{\text{radial eigenfunctions}} \overbrace{Y_{lm}(\theta,\varphi)}^{\text{spherical harmonics}}$$

- The radial eigenfunctions obey the differential equation (radial equation):

$$\left[-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{\hbar\, \ell(\ell+1)}{2\mu r^2} + U(r)\right]R(r) = E_k\, R(r).$$

- Since we are dealing with elastic scattering, the energy $E_k = \frac{\hbar k^2}{2\mu} > 0$ is fixed.
- Since, k and ℓ appear in the above equation, we write $R(r) = R_{k,\ell}(r)$.
- Let us first consider the case $U(r)=0$, which describes the situation long before and after the scattering event:

$$\hookrightarrow \left[\frac{1}{r}\frac{d^2}{dr^2}r + k^2 - \frac{\ell(\ell+1)}{r^2}\right]R_{k,\ell}(r) = 0 \quad , \quad \text{or}$$

$$r^2 R''_{k,\ell} + 2r R'_{k,\ell} + (k^2 r^2 - \ell(\ell+1))\, R_{k,\ell} = 0 .$$

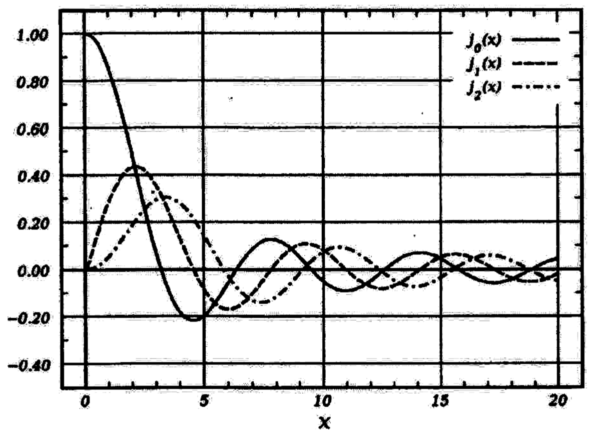
- This equation is known as <u>Bessel differential equation</u>.
- Its solutions are given by the <u>spherical Bessel functions</u>.

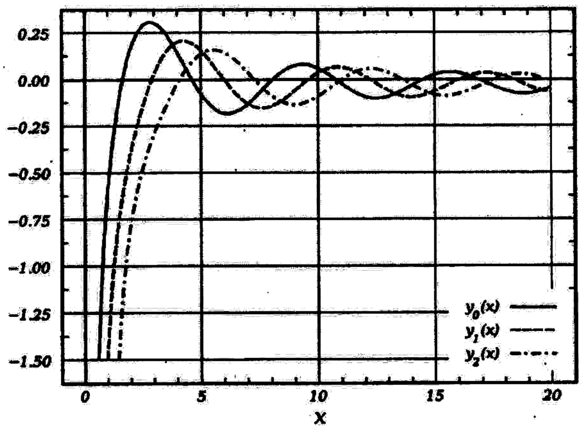
$$j_\ell(x) = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x}$$

$$y_\ell(x) = -(-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x} \quad \Big\} \text{ often also referred to as spherical Neumann functions}$$

- The general solution of the free ($U(r)=0$) stationary Schrödinger equation is a superposition of terms proportional to $j_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$ and $y_\ell(kr)\, Y_{\ell m}(\theta,\varphi)$, for all ℓ and m.

Spherical Bessel and Neumann functions





$$j_0(x) = \frac{\sin x}{x}, \qquad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \qquad j_2(x) = \left(\frac{3}{x^2} - 1\right)\frac{\sin x}{x} - \frac{3\cos x}{x^2}$$

$$y_0(x) = -\frac{\cos x}{x}, \qquad y_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}, \qquad y_2(x) = \left(-\frac{3}{x^2} + 1\right)\frac{\cos x}{x} - \frac{3\sin x}{x^2}$$

Wikipedia

- The functions $y_\ell(x)$ diverge at $x=0$.
- For problems for which one is interested in the behaviour of the wave functions at the origin, the $y_\ell(x)$ must be discarded, since they cannot be normalised.
- The asymptotic behaviour of the Bessel functions for large $x = kr$ is given by

$$j_\ell(x) \overset{x\gg 1}{\approx} \frac{\sin\left(x - \ell\frac{\pi}{2}\right)}{x}$$

$$y_\ell(x) \overset{x\gg 1}{\approx} -\frac{\cos\left(x - \ell\frac{\pi}{2}\right)}{x}$$

- To see how this result is obtained, consider

$$j_\ell(x) = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x} = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^{\ell-1}\left(\frac{\cos x}{x^2} - \frac{\sin x}{x^3}\right).$$

- The leading term (with the lowest power of $\frac{1}{x}$) is alternating between sin and cos, and with every differentiation its power increases by one.

$\hookrightarrow$ $$j_\ell(x) \overset{x\gg 1}{\approx} (-x)^\ell \frac{1}{x^{\ell+1}} \frac{d^\ell}{dx^\ell} \sin x = (-1)^\ell \frac{1}{x} (-1)^\ell \sin\left(x - \ell\frac{\pi}{2}\right)$$

$$= \frac{\sin\left(x - \ell\frac{\pi}{2}\right)}{x}$$

- A similar reasoning yields the asymptotic behaviour of the y_ℓ.

- For a spherically symmetric scattering potential the scattering amplitude does not depend on the azimuthal angle φ.
- (Note, that the $\vec{k}$ vector of the incoming particle is aligned with the z-axis.)
- This symmetry restricts the set of spherical harmonics which are required to describe the scattering process to

$$\underbrace{Y_{l0}}_{\text{azimuthal quantum number is set to zero}}(\theta,\varphi) = \overbrace{\sqrt{\frac{2l+1}{4\pi}}\; P_l(\cos\theta)}^{\text{no } \varphi\text{-dependence}} .$$

- Here, the P_l are the Legendre polynomials

$$P_l(\cos\theta) = \frac{(-1)^l}{2^l l!} \frac{d^l}{d\cos\theta^l} \sin^{2l}\theta .$$

- One can show that a plane wave can actually be expanded in terms of Bessel functions and Legendre polynomials:

$$\underbrace{e^{ikz}}_{\substack{\text{incoming } \vec{k} \\ \text{is aligned} \\ \text{with } z\text{-axis}}} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l (2l+1)\, j_l(kr)\, P_l(\cos\theta)$$

- We are now considering the asymptotic form of this expression, far away from the scattering centre:

$$e^{ikz} \approx \sum_{\ell=0}^{\infty} i^{\ell}(2\ell+1) \overbrace{\frac{\sin\left(kr - \ell\frac{\pi}{2}\right)}{kr}}^{\text{asymptotics of } j_\ell} P_\ell(\cos\theta)$$

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2ikr}\left[i^{\ell} e^{ikr} e^{-i\ell\frac{\pi}{2}} - i^{\ell} e^{-ikr} e^{i\ell\frac{\pi}{2}}\right] P_\ell(\cos\theta)$$

$$= \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2ikr}\left[e^{ikr} - (-1)^{\ell} e^{-ikr}\right] P_\ell(\cos\theta)$$

- In the next step we take a look at the general scattering solution

$$u_k(\vec{r}) = e^{ikz} + f_k(\theta)\,\frac{e^{ikr}}{r}.$$

- Also the scattering amplitude $f_k(\theta)$ can also be expanded in terms of Legendre polynomials

$$f_k(\theta) = \sum_{\ell=0}^{\infty} \underbrace{(2\ell+1)}_{\substack{\text{it turns out}\\ \text{to be convenient}\\ \text{to have this}\\ \text{factor}}} \underbrace{f_{k,\ell}}_{\substack{\text{expansion coefficients,}\\ \text{also called partial}\\ \text{wave amplitudes.}}} P_\ell(\cos\theta)$$

- Plugging this expression and the expansion of the plane wave into the scattering solution yields

$$u_k(\vec{r}) = \sum_{l=0}^{\infty} \frac{2l+1}{2ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right] P_l(\cos\theta) + \frac{e^{ikr}}{r}\sum_{l=0}^{\infty}(2l+1) f_{k,l} P_l(\cos\theta)$$

$$= \sum_{l=0}^{\infty}(2l+1) P_l(\cos\theta) \frac{e^{ikr}\overbrace{(1+2ik f_{k,l})}^{S_l} - (-1)^l e^{-ikr}}{2ikr}$$

$$= \sum_{l=0}^{\infty}(2l+1) P_l(\cos\theta) \frac{e^{ikr} S_l - (-1)^l e^{-ikr}}{2ikr}$$

- The factor S_l is called <u>scattering matrix element</u>.

- The reason for this name is that in a general (non-spherically symmetric) scattering potential the so-called scattering matrix (or S-matrix) $S_{ll'}$ appears, which depends on the incoming and outgoing angular momenta l, l'.

- As previously discussed, the radial component j_r of the probability current has to vanish when integrating over a spherical shell with radius r around the scatterer.

- This has to hold for all l-components

$$u_{k,l}(r) = (2l+1) P_l(\cos\theta) \frac{e^{ikr} S_l - (-1)^l e^{-ikr}}{2ikr}$$

separately

- For the radial current one finds

$$\int d\Omega \, j_{r,\ell} = \int d\Omega \frac{\hbar}{2\mu i}\left(u^*_{k,\ell}\frac{du_{k,\ell}}{dr} - \frac{du^*_{k,\ell}}{dr}u_{k,\ell}\right)$$

$$= \frac{(2\ell+1)\hbar}{\mu k r^2}\left(|S_\ell|^2 - 1\right) \stackrel{!}{=} 0 .$$

- Hence, we find that $|S_\ell| = 1$ and thus the scattering matrix element can be parametrized as

$$S_\ell = e^{2i\delta_\ell} , \qquad \left(-\frac{\pi}{2} \le \delta_\ell \le \frac{\pi}{2}\right)$$

where δ_ℓ is the <u>scattering phase</u>, which depends on ℓ as well as on the momentum k.

- Using δ_ℓ, we can write the scattering state as

$$u_\ell(\vec{r}) = \sum_{\ell=0}^{\infty}(2\ell+1)P_\ell(\cos\theta)\,\frac{e^{i(kr+2\delta_\ell)} - (-1)^\ell e^{-ikr}}{2ikr} ,$$

which is the so-called <u>partial wave decomposition</u>.

- From this expression it becomes apparent, that the outgoing spherical wave, e^{ikr}, acquires a phase shift of $2\delta_\ell$, in which the information about the scatterer is contained.

- We can now write (p. 164)

$$f_{k,\ell} = \frac{S_\ell - 1}{2ik} = \frac{e^{2i\delta_\ell} - 1}{2ik} = \frac{e^{i\delta_\ell}}{k} \sin \delta_\ell ,$$

and inserting this into the expansion of the scattering amplitude yields

$$f_k(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \underbrace{e^{i\delta_\ell} \sin \delta_\ell}_{\substack{\text{scattering phases} \\ \text{determine scattering} \\ \text{amplitude}}} P_\ell(\cos\theta) .$$

- The differential scattering cross section is defined as

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

and it will in general have a complicated shape due to the interference of many partial wave components.

- For the total cross section one obtains

$$\sigma = \int d\Omega \, |f_k(\theta)|^2 = \frac{1}{k^2} \int d\Omega \sum_{\ell,\ell'=0}^{\infty} (2\ell+1)(2\ell'+1) e^{i\delta_\ell} e^{i\delta_{\ell'}} \sin\delta_\ell \sin\delta_{\ell'} P_\ell(\cos\theta) P_{\ell'}(\cos\theta) ,$$

which simplifies drastically after using the orthogonality relation of the Laguerre polynomials

$$\int d\Omega \; P_\ell(\cos\theta) P_{\ell'}(\cos\theta) = 2\pi \, \delta_{\ell\ell'} \frac{2}{2\ell+1} .$$

$$\hookrightarrow \quad \sigma = \sum_{\ell=0}^{\infty} \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell = \sum_{\ell=0}^{\infty} \sigma_\ell$$

knowledge of the scattering phases solves the scattering problem

each partial wave yields a separate contribution to the scattering cross section

- The partial wave decomposition also leads to the optical theorem:

$$\mathrm{Im}\left[f_k(\theta)\right] = \sum_{\ell=0}^{\infty}(2\ell+1)\frac{\sin^2\delta_\ell}{k}P_\ell(\cos\theta),$$

which for $\theta = 0$ becomes (using $P_\ell(1)=1$)

$$\mathrm{Im}\left[f_k(0)\right] = \sum_{\ell=0}^{\infty}(2\ell+1)\frac{\sin^2\delta_\ell}{k} = \frac{k}{4\pi}\sigma$$

$$\hookrightarrow \quad \sigma = \frac{4\pi}{k}\mathrm{Im}\left[f_k(\theta=0)\right]$$

- The total cross section associated with a certain ℓ-value is proportional to $\sin^2\delta_\ell$ and thus becomes maximal for $\delta_\ell = \pm\frac{\pi}{2}$.

- Such maximum is associated with a <u>scattering resonance</u> as we will show in the following for $\delta_\ell = +\frac{\pi}{2} \equiv \delta_\ell^{R}$ (R = resonance).

- To investigate the behaviour of the partial wave amplitude near such resonance, we write it as

$$f_{k,\ell} = \frac{\sin\delta_\ell}{k(\cos\delta_\ell - i\sin\delta_\ell)} = \frac{\tan\delta_\ell}{k(1-i\tan\delta_\ell)} .$$

- For $\delta_\ell = \delta_\ell^R = \frac{\pi}{2}$ one finds

$$f_{k,\ell}^R \equiv f_{k,\ell}(\delta_\ell^R) = -\frac{1}{ik},$$

since

$$\lim_{\delta_\ell \to \delta_\ell^R} \tan\delta_\ell = \infty .$$

- In the vicinity of δ_ℓ^R we can expand the tangens into a Laurent series:

$$\tan\delta_\ell = -\frac{1}{\delta_\ell - \delta_\ell^R} + \mathcal{O}(1) .$$

- Next, we consider that the scattering phase δ_ℓ is a function of energy, i.e. $\delta_\ell(E)$, and we denote as E_ℓ^R the energy at which $\delta_\ell(E_\ell^R) = \delta_\ell^R = \frac{\pi}{2}$.
- Expanding around E_ℓ^R yields:

$$\delta_\ell(E) = \underbrace{\delta_\ell^R}_{\delta_\ell(E_\ell^R)} + \delta_\ell'(E_\ell^R)(E - E_\ell^R) + \mathcal{O}((E-E_\ell^R)^2) .$$

- Defining $\Gamma_\ell = -\dfrac{2}{\delta_\ell'(E_\ell^R)}$ we can write

$$\tan\delta_\ell \approx \frac{\frac{\Gamma_\ell}{2}}{E - E_\ell^R}$$

and the partial wave amplitude becomes

$$f_{k,\ell} = \frac{1}{k}\,\frac{\frac{1}{2}\Gamma_\ell}{E - E_\ell^R - i\frac{1}{2}\Gamma_\ell}$$

- The contribution of this partial wave to the total scattering cross section thus becomes

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell \overset{\text{p.166}}{=} \frac{4\pi}{k^2}(2\ell+1)\,k^2\sin^2\delta_\ell$$

$$= \frac{4\pi}{k^2}(2\ell+1)\,\frac{\frac{1}{4}\Gamma_\ell^2}{(E-E_\ell^R)^2 + \frac{1}{4}\Gamma_\ell^2}.$$

- This is a Breit-Wigner profile with width Γ_ℓ.
- Such resonances are related to the emergence of bound states, such as the (temporary) creation of new particles, during a scattering process.

- We conclude this chapter by discussion some properties of the scattering phases for spherically symmetric potentials that vanish outside a given radius r_0:

$$V(r) = \begin{cases} W(r) & , r \leq r_0 \\ 0 & , r > r_0 . \end{cases}$$

- For $r > r_0$ the solution of the radial Schrödinger equation is

$$R_{k,\ell}(r) = \underset{\uparrow}{a}\, j_\ell(kr) + \underset{\uparrow}{b}\, y_\ell(kr) .$$

complex coefficients

- It is now convenient to introduce the so-called spherical Hankel functions

$$h_\ell(kr) = j_\ell(kr) + i\, y_\ell(kr)$$
$$h_\ell^*(kr) = j_\ell(kr) - i\, y_\ell(kr),$$

which allows us to write

$$R_{k,\ell}(kr) = A\, h_\ell(kr) + B\, h_\ell^*(kr)$$

- For large r we find the asymptotic behaviour

$$h_\ell(kr) \overset{kr \gg 1}{\approx} \frac{\sin(kr - \ell\frac{\pi}{2})}{kr} - i\, \frac{\cos(kr - \ell\frac{\pi}{2})}{kr} = \frac{e^{i(kr - \ell\frac{\pi}{2})}}{ikr}$$

and thus

$$R_{k\ell}(r) \overset{kr \gg 1}{\approx} \frac{A e^{i(kr - \frac{\pi}{2}\ell)} - B e^{-i(kr - \frac{\pi}{2}\ell)}}{ikr} = B e^{-i\ell\frac{\pi}{2}}\, \frac{\frac{A}{B} e^{ikr} - (-1)^\ell e^{-ikr}}{ikr} .$$

- In order for this to be a scattering solution we must require $\frac{A}{B} = e^{2i\delta_\ell}$ and thus we find for $r > r_0$ the radial solution

$$R_{k,\ell}(r) = B\left(h_\ell(kr)\, e^{2i\delta_\ell} + h_\ell^*(kr)\right).$$

- This solution has to be matched with the the solution $\bar{R}_{k\ell}$ inside the region $r \le r_0$.
- At the matching point r_0 both logarithmic derivatives have to be equal:

$$\alpha_\ell \equiv \frac{\bar{R}'_{k,\ell}(r_0)}{\bar{R}_{k,\ell}(r_0)} = k\, \frac{h_\ell'(kr_0)\, e^{2i\delta_\ell} + h_\ell^{*\prime}(kr_0)}{h_\ell(kr_0)\, e^{2i\delta_\ell} + h_\ell(kr_0)}.$$

value of the logarithmic derivative of $\bar{R}_{k\ell}$ at $r = r_0$.

- Solving for the scattering phases δ_ℓ yields

$$\tan\delta_\ell = \frac{k\, j_\ell'(kr_0) - \alpha_\ell\, j_\ell(kr_0)}{k\, Y_\ell'(kr_0) - \alpha_\ell\, Y_\ell(kr_0)}.$$

- For a hard sphere potential, i.e. $W(r) \to \infty$, one has $\bar{R}_{k,\ell}(r_0) \to 0$ and thus $\alpha_\ell \to \infty$.
- This yields for the scattering phase shifts

$$\tan\delta_\ell = \frac{j_\ell(kr_0)}{Y_\ell(kr_0)}$$

which for $\ell = 0$ leads to $\delta_0 = -kr_0$.

- This is a manifestation of a more general result, namely that the scattering phases become negative for a repulsive potential.

- Let us now return to the general expression for $\tan\delta_\ell$ and investigate it for small energies, i.e. $k \to 0$.

- Using the expansion

$$j_\ell(x) \overset{x \ll 1}{\approx} \frac{x^\ell}{(2\ell+1)!!}, \quad y_\ell(x) \overset{x \ll 1}{\approx} - x^{-\ell-1}(2\ell+1)!!$$

yields

$$\tan\delta_\ell \sim k^{2\ell+1}$$

for $k \to 0$.

- The scattering phase thus decreases with k, and the larger ℓ the faster this decrease becomes.

- For sufficiently small energy the dominant contribution to the scattering thus comes from the $\ell=0$ component, which is referred to <u>s-wave scattering</u>.

- In this case

$$\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2 = \frac{\sin^2\delta_0}{k^2} \overset{\delta_0 \sim k}{\sim} \text{const.}$$

does not depend on energy

- One can now define the so-called s-wave <u>scattering length</u> a_s:

$$\lim_{k \to 0} k \cdot \cot(\delta_0) = -\frac{1}{a_s}.$$

- With this definition, the scattering cross section becomes at low energies

$$\sigma = 4\pi a_s^2,$$

and for a hard sphere of radius r_0 one finds $a_s = r_0$.

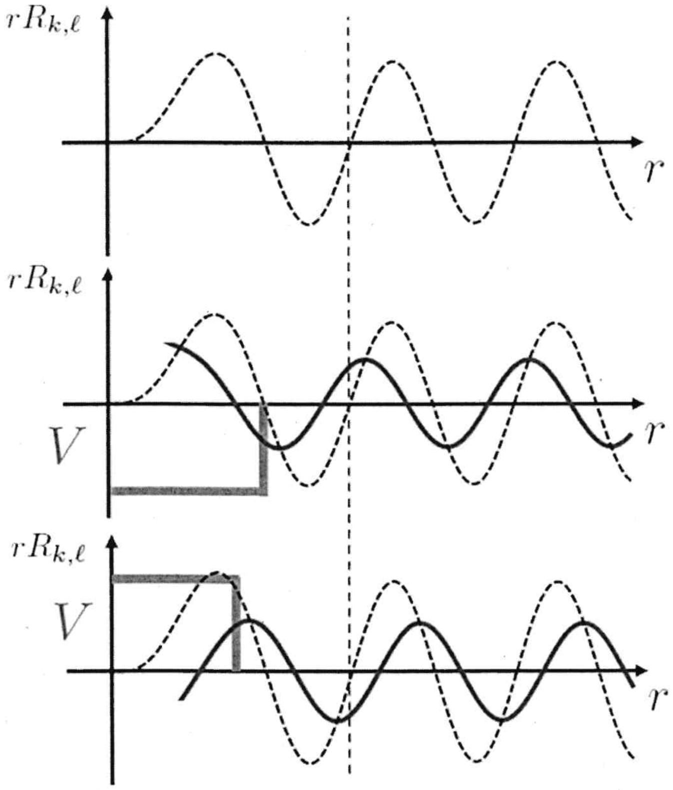
- The s-wave scattering length is positive for repulsive potentials.
- For attractive potentials it is negative, but can also become positive, when the potential permits bound states.
- To see this lets consider an attractive potential, $W(r) = -W$, which has a bound state close to $E = 0$ (bound state energy: $E_B < 0$)
- The associated radial wave function is

$$R_{k,l=0}(r) \sim \frac{e^{-\kappa r}}{\kappa r},$$

with $\frac{\hbar^2 \kappa^2}{2\mu} = E_B$.

- This solution corresponds to a scattered wave function with $k = i\kappa$.

Qualitative behaviour of the scattering phase



$V = 0 \rightarrow \delta = 0$

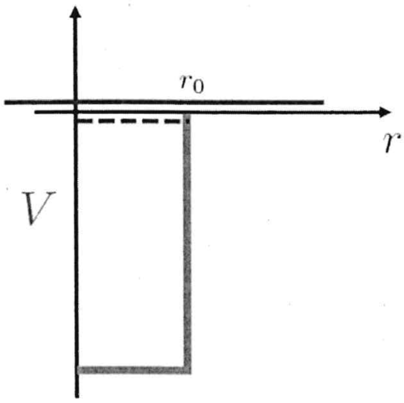
attractive potential

$\delta > 0$

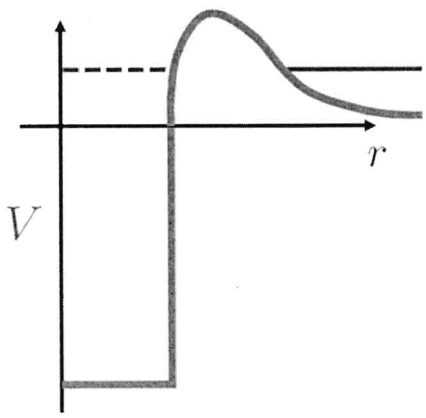
repulsive potential

$\delta < 0$

Bound state



Metastable state



Skript zur Vorlesung
Fortgeschrittene Quantentheorie
(Quantenmechanik II)
Prof. Werner Vogelsang
Universität Tübingen
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- Evaluating the scattering phase shift by matching the logarithmic derivatives at r_0, yields

$$\tan \delta_0 = -i ,$$

and hence

$$e^{2i\delta_0} = - \frac{(\tan \delta_0 - i)^2}{1 + \tan^2 \delta_0} = \infty$$

↳ the scattering matrix element has a pole in the complex plane, which corresponds to the bound state.

- Generally, one finds for the behaviour of the total scattering cross section in the vicinity of a bound state

$$\sigma = \frac{2\pi\hbar^2}{\mu} \frac{1}{E - E_B} .$$