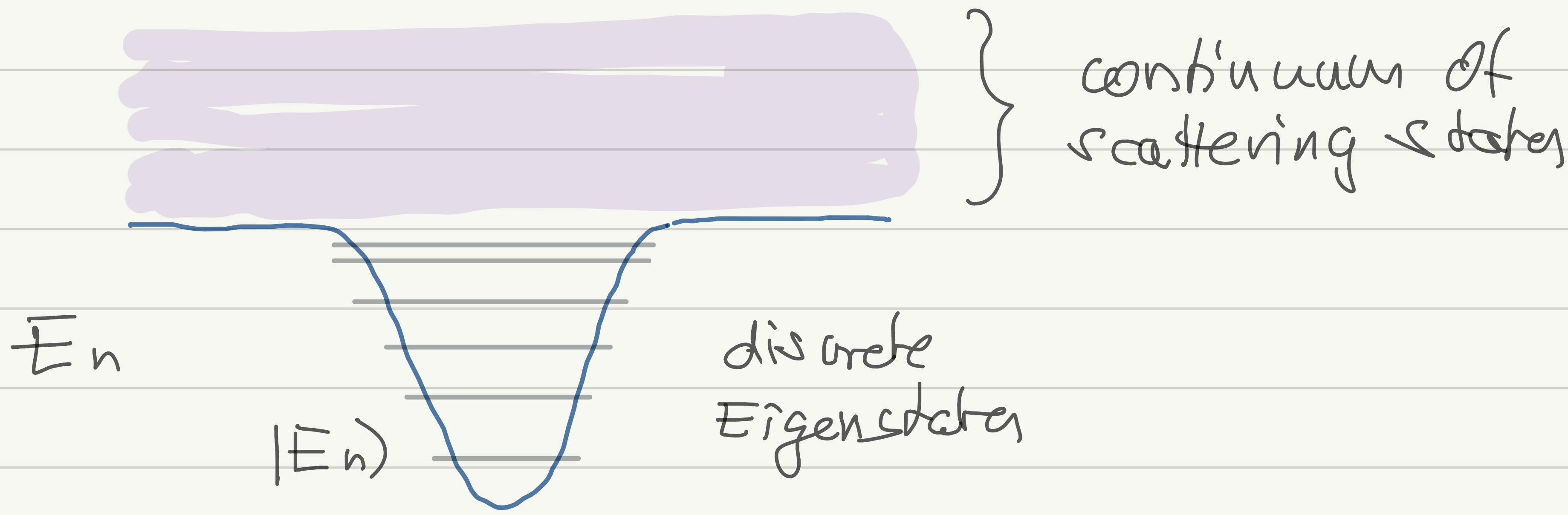
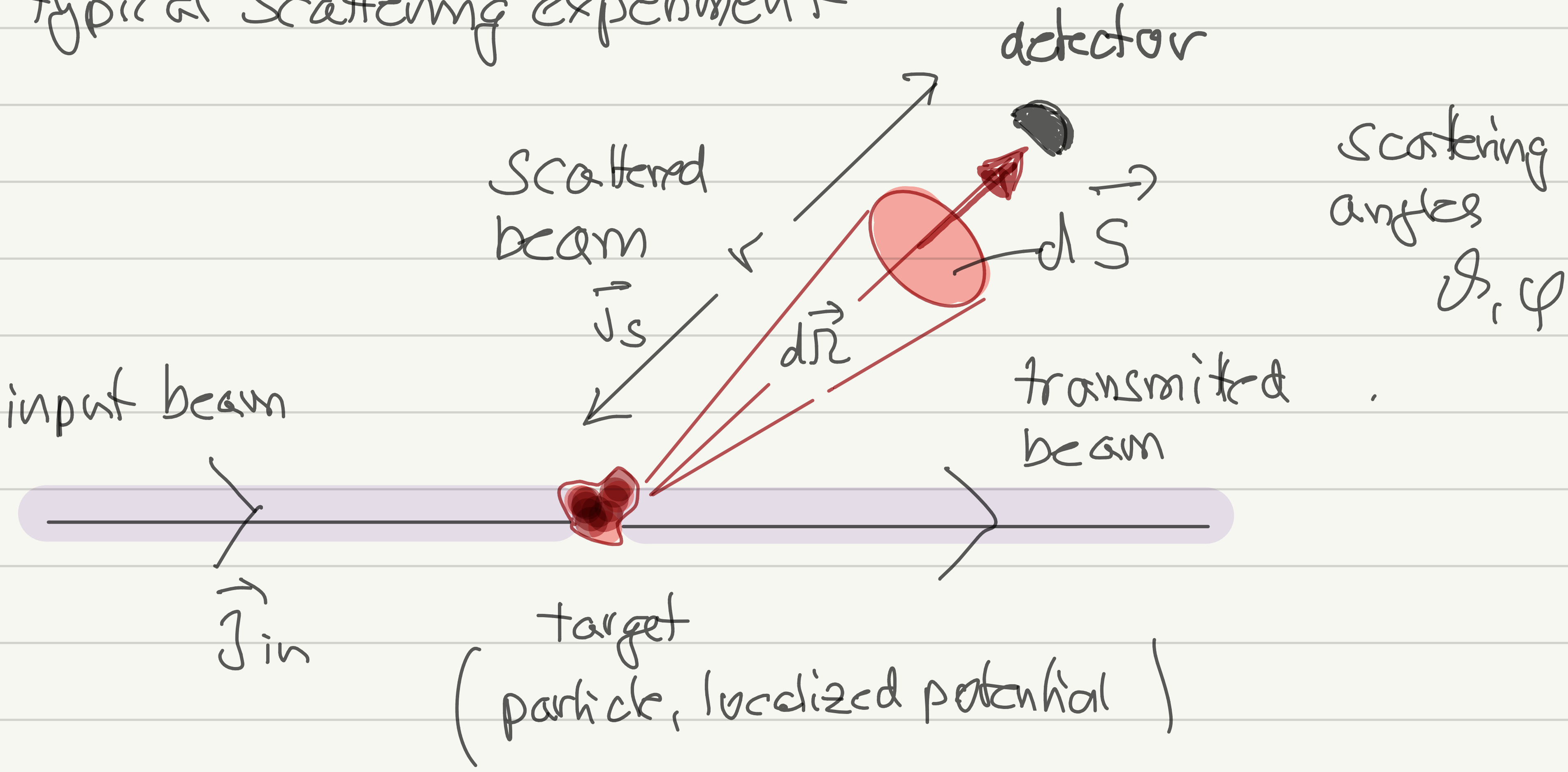
III. Scattering theory

In the quantum mechanics lecture we have so far mostly discussed discrete eigenstates of quantum systems. Often the physics involving the continuum of scattering states is however as important



III.1 Basic concepts

typical scattering experiment



Solid angle of scattering

$$d\vec{\Omega} = \vec{n}\, d\Omega$$

detector area

$$d\vec{S} = r^2 d\vec{\Omega}$$

number of particles going through $d\vec{S}$ per unit of time

$$(104) \qquad dN = \vec{j}_s \cdot d\vec{S} = \vec{j}_s \cdot \vec{n}\, r^2 d\Omega$$

differential scattering cross section

$$(105) \qquad \boxed{d\sigma = \frac{dN}{|\vec{j}_{in}|} = \frac{r^2\, j_{s,r}}{|\vec{j}_{in}|}\, d\Omega} \Rightarrow \frac{d\sigma}{d\Omega}$$

total scattering cross section

$$(106) \qquad \boxed{\sigma = \int d\Omega\, \frac{d\sigma}{d\Omega}}$$

scattering amplitude

Assume the target is a potential $V(\vec{r})$ centered at $\vec{r}=0$ and $V(\vec{r})$ has finite range; i.e it decays faster than $1/r$.

$\Rightarrow$ input and scattered states are solutions of the free Schrödinger equation

(107) $$H = \frac{\hat{\vec{P}}^2}{2m}, \quad \vec{P} \text{ fixed say in } z \text{ direction}$$

$$\Rightarrow \quad \varphi_{in}(\vec{r}) \sim e^{ikz} \qquad E_k = \frac{\hbar^2 k^2}{2m}$$

asymptotics of scattered wavefunction

<u>(i) isotropic scattering</u> $\qquad P_\varphi = P_\vartheta = 0$

$\qquad P_r \neq 0$

$\Rightarrow$

(108) $$\frac{\hat{P}_r^2}{2m} \varphi_k(\vec{r}) = E_k \varphi_k(\vec{r})$$

Solution, see QMI $\quad$ spherical Besselfunction

$$\varphi_k(\vec{r}) = \varphi_k(r) = j_0(kr) = \frac{\sin kr}{kr}$$

$$= \frac{1}{2i}\left(\frac{e^{ikr}}{kr} - \frac{e^{-ikr}}{kr}\right)$$

(109) $$\Rightarrow \quad \varphi_k(r) \sim \frac{e^{ikr}}{r} \qquad \text{for isotropic scattering}$$

<u>(ii) general case: anisotropic scattering</u>

(110) $$\boxed{\varphi_k(r,\vartheta,\varphi) \sim f_k(\vartheta,\varphi)\frac{e^{ikr}}{r}} \qquad r \to \infty$$

$f_k(\vartheta,\varphi)$ is called scattering amplitude

If the target is a central potential the scattering problem has cylinder symmetry and

(111) $$f_k(\vartheta,\varphi) \longrightarrow f_k(\vartheta)$$

relation between scattering amplitude and differential cross section

$$\vec{j}_s = \frac{\hbar}{2mi}\left(\phi_s^*(\vec{r})\,\vec{D}\,\phi_s(\vec{r}) - \phi_s(\vec{r})\,\vec{D}\,\phi_s^*(\vec{r})\right)$$

$$\vec{j}_s\cdot\vec{e}_r = \frac{\hbar}{2mi}\left(\phi_s^*\frac{\partial}{\partial r}\phi_s - \phi_s\frac{\partial}{\partial r}\phi_s^*\right)$$

(112) $$\underset{r\to\infty}{=} \frac{\hbar k}{m r^2}\,|f_k(\vartheta,\varphi)|^2$$

on the other hand the current of the incoming particles is

(113) $$\vec{j}_{in} = \frac{\hbar k}{m}\,\vec{e}_z$$

(114) $$\boxed{\frac{d\sigma}{d\Omega} = \frac{r^2\, j_{s,r}}{|\vec{j}_{in}|} = |f_k(\vartheta,\varphi)|^2}$$

III.2 Scattering of a central potential
partial wave decomposition

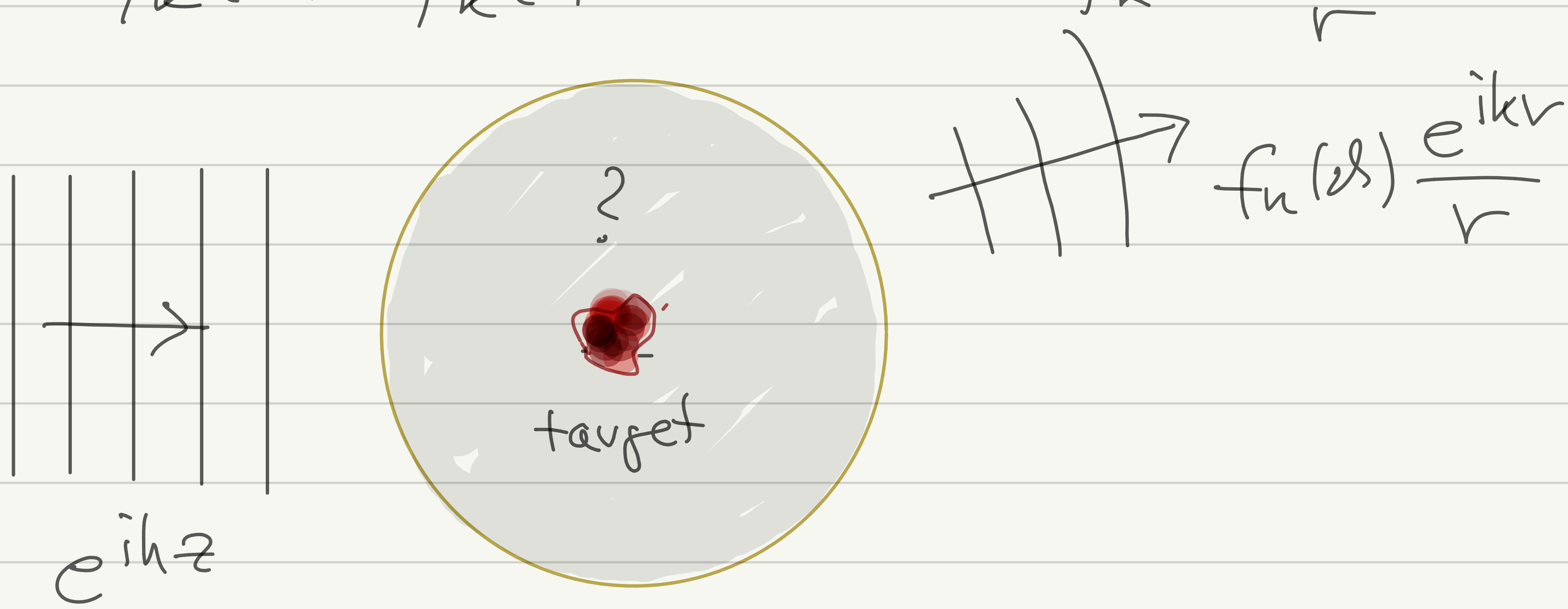
Of particular importance is the scattering of a central potential

$$\boxed{\begin{aligned} &V(\vec{r}) = V(r) \\ \text{with} \quad &(i) \quad rV(r) \to M \quad \text{for } r \to 0 \\ (115) \quad &(ii) \quad \lim_{r\to\infty} r^{1+\varepsilon} V(r) = 0 \quad \varepsilon > 0 \end{aligned}}$$

Remark: conditions not fulfilled for Coulomb potential
→ needs separate discussion

The asymptotic form of the wavefunction (without normalization) i.e. far away from the scattering center for initial momentum $\hbar\vec{k} = \hbar k\vec{e}_z$

$$(116) \quad \varphi_k(\vec{r}) = \varphi_k(r,\vartheta) = e^{ikz} + f_k(\vartheta)\frac{e^{ikr}}{r}$$



▶ for $V=0$ φ_k is solution of stationary radial Schrödinger equation, so

(117) $$\varphi_k(r,\vartheta) = \sum_{\ell=0}^{\infty} c_\ell \, R_{k\ell}(r) \, P_\ell(\cos\vartheta)$$

Legendre polynomials

and

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

This equation has been discussed in QM I. The solutions are spherical Bessel functions

(119) $$R_{k\ell}(r) \sim j_\ell(kr)$$

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

for $x \to \infty$

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

i.e.

(120) $$R_{k\ell}(r) \xrightarrow[r\to\infty]{} \frac{1}{kr}\sin\left(kr - \frac{\ell\pi}{2}\right)$$

▶ for $V \neq 0$ we expect the same asymptotic form apart from a possible phase shift

$$(121) \quad \boxed{\varphi_k(r,\vartheta) = \sum_{\ell=0}^{\infty} C_\ell \frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)}{kr} P_\ell(\cos\vartheta)}$$

partial wave decomposition of scattering wavefunction

δ_ℓ – scattering phase

relation between scattering amplitudes and scattering phases

eq. (121) ⇔ (116)

$$\underset{\text{input wave}}{e^{ikz}} = e^{ikr\cos\vartheta} \underset{\substack{\uparrow \\ \text{homework problem}}}{=} \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell j_\ell(kr) P_\ell(\cos\vartheta)$$

$$(122) \quad \xrightarrow[r\to\infty]{} \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell \frac{\sin\left(kr - \frac{\ell\pi}{2}\right)}{kr} P_\ell(\cos\vartheta)$$

total wave

$$e^{ikz} + f_k(\vartheta) \frac{e^{ikr}}{r} =$$

$$= \sum_{\ell=0}^{\infty} (2\ell+1) i^\ell \frac{\sin(kr - \frac{\ell\pi}{2})}{kr} P_\ell(\cos\vartheta)$$

(123) $$+ f_k(\vartheta) \frac{e^{ikr}}{r}$$

$$\overset{!}{=} \sum_{\ell=0}^{\infty} c_\ell \frac{\sin(kr - \frac{\ell\pi}{2} + \delta_\ell)}{kr} P_\ell(\cos\vartheta)$$

$\Rightarrow \ldots \Rightarrow$

(124)
$$\boxed{\begin{aligned} c_\ell &= i^\ell (2\ell+1) e^{i\delta_\ell} \\ f_k(\vartheta) &= \frac{1}{k} \sum_{\ell=0}^{\infty} \frac{c_\ell}{i^\ell} \sin\delta_\ell \, P_\ell(\cos\vartheta) \end{aligned}}$$

partial-wave decomposition of scattering amplitude

using the orthogonality of the Legendre polynomials $P_\ell(\cos\vartheta)$ one finds for the total cross section

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

setting $\vartheta = 0$ in (124)

$$f_k(0) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \sin\delta_\ell \cos\delta_\ell + \frac{i}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2\delta_\ell$$

this yields

$$\boxed{\sigma = \frac{4\pi}{k} \, \mathrm{Im}\left[f_k(\vartheta=0) \right]} \tag{126}$$

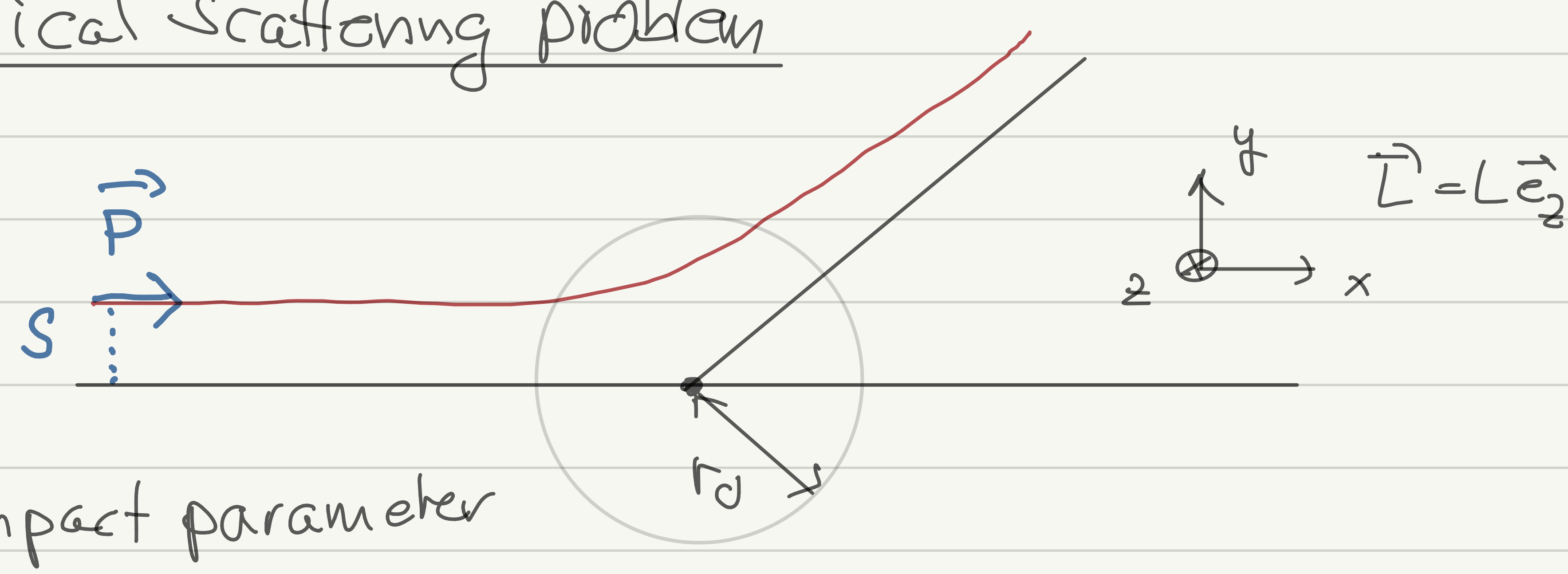
optical theorem

which establishes a connection between the total cross section and the imaginary part of the forward scattering amplitude!

III.3 Low-energy scattering

We will see now that the partial wave decomposition of the scattering amplitude is particularly useful for scattering processes at low energy

classical scattering problem



s - impact parameter

angular momentum with respect to scattering center $\qquad L = sp$

If scattering potential negligible for $r > r_0$

$\Rightarrow$ only effect if $\quad L < r_0 p$

quantum mechanical scattering problem

$$L = \hbar\sqrt{l(l+1)} \sim \hbar l \qquad p = \hbar k$$

$\Rightarrow$ only scattering for $\quad \hbar l < r_0 \hbar k$

(127) $$\boxed{l < r_0 k}$$

for very low energies ($k^2/2m$) only $l=0$ term relevant

s-wave scattering

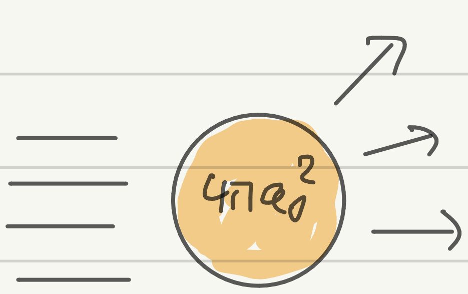
s-wave scattering approximation

(128) $$\boxed{f_k(\vartheta) = \frac{1}{k} e^{i\delta_0} \sin\delta_0}$$ isotropic

(129) $$\boxed{\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\sin^2\delta_0 \simeq \frac{\delta_0^2}{k^2}}$$

s-wave scattering length

(130) $$\boxed{\frac{d\sigma}{d\Omega} \stackrel{!}{=} a_0^2 \qquad \sigma = 4\pi a_0^2}$$



from (128)

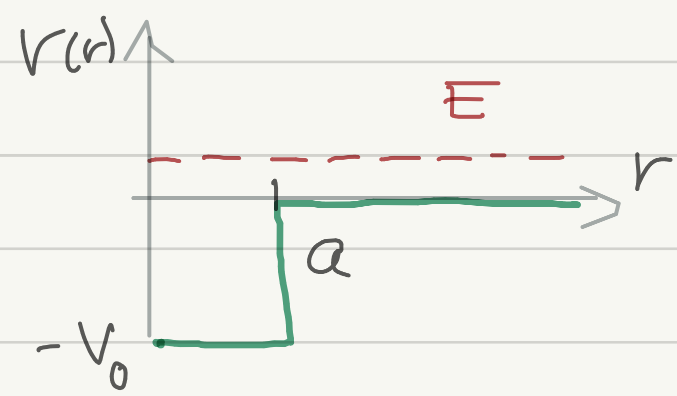
(131) $$\boxed{a_0 \equiv -\lim_{k\to 0} f_k(\vartheta) \simeq -\lim_{k\to 0} \frac{\delta_0}{k}}$$

<u>s-wave scattering length</u>

Low-energy scattering at a local potential $V(r)$ of otherwise arbitrary shape can be fully desribed by a single parameter a_0 (or equivalently δ_0)

<u>Example 1:</u> Scattering off an attractive spherical potential well

(132) $$V(r) = \begin{cases} -V_0 & r < a \\ 0 & r > a \end{cases}$$



low-energy scattering only $l=0$ in radial Schrö-dinger equation

(133) $$\left[\frac{1}{r}\frac{d^2}{dr^2} r + k^2 - \frac{2mV(r)}{\hbar^2}\right] R_{k0}(r) = 0$$

$\boxed{r < a}$ $$\frac{\hbar^2 k_1^2}{2m} = E + V_0$$ $$E = \frac{\hbar^2 k^2}{2m}$$ incoming particle

define $u_1 = rR$

$$\frac{d^2 u_1}{dr^2} + k_1^2 u_1 = 0 \quad \Rightarrow \quad \underline{\underline{u_1 = A \sin k_1 r}} \quad (134)$$

$\boxed{r > a}$ asymptotic solution from (121) and $l = 0$

$$(135) \qquad \underline{\underline{u_2 = B \sin(kr + \delta_0)}} \qquad E = \frac{\hbar^2 k^2}{2m}$$

boundary conditions at $r = a$

$$\hat{p}_r^{\,2} R(r) = \frac{-\hbar^2}{r} \frac{\partial}{\partial r}\left[\frac{\partial}{\partial r} u\right]$$

$\Rightarrow$ u continuous ! $\quad \frac{\partial u}{\partial r}$ continuous

$\frac{d \ln u}{dr}$ continuous at $r = a$

this yields

$$k \to 0 \quad \delta_0 \to 0$$

$$(136) \quad k_1 \cot k_1 a = k \cot(ka + \delta_0) \simeq \frac{k}{ka + \delta_0}$$

$$\Rightarrow$$

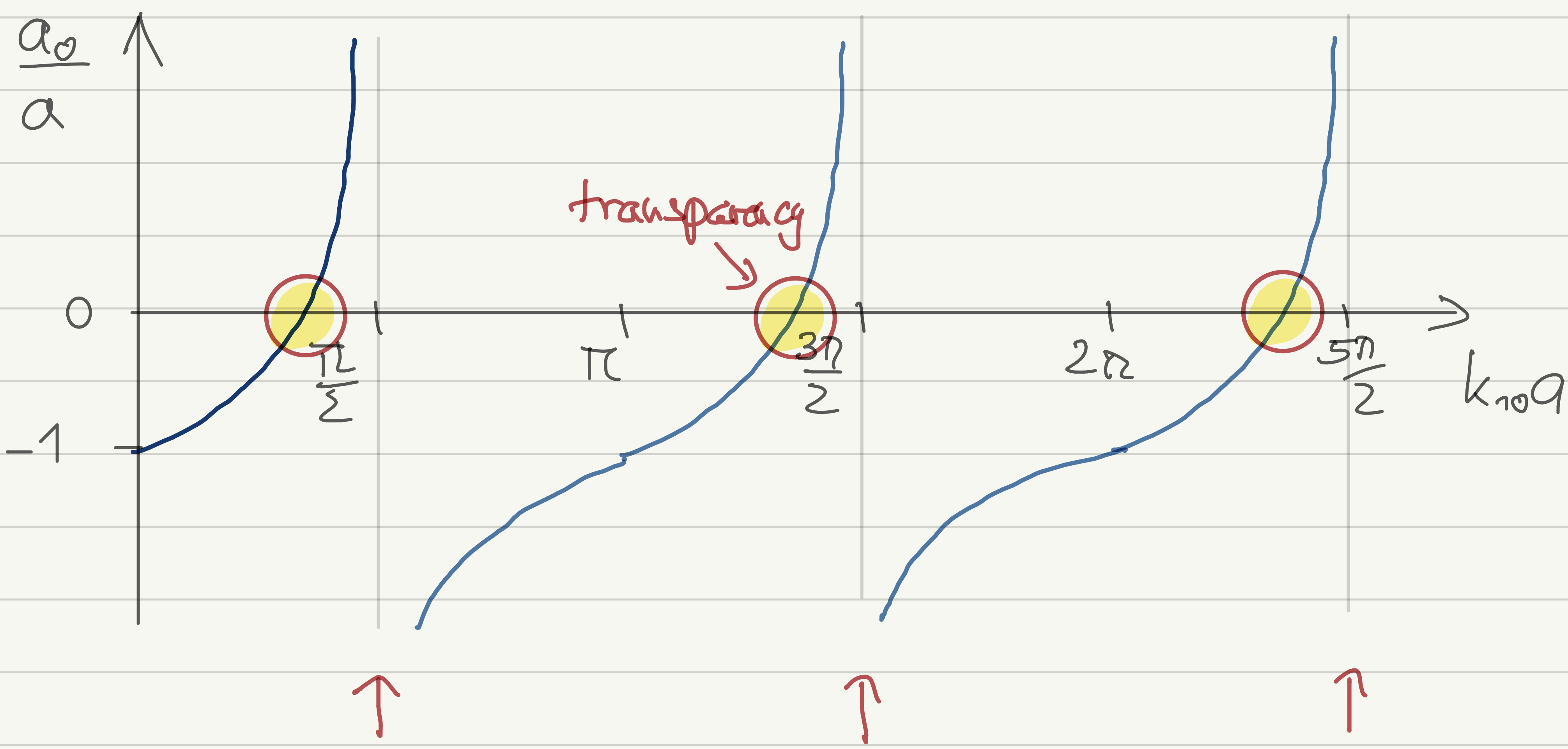
$$(137) \qquad \underline{\underline{\delta_0 = ka\left(\frac{\tan k_1 a}{k_1 a} - 1\right)}}$$

s-wave scattering length

$$(138) \qquad \underline{\underline{a_0 = a\left(\frac{\tan k_{10} a}{k_{10} a} - 1\right)}} \qquad k_{10} = \lim_{k \to 0} k_1$$

where $\quad k_{10} = \frac{\sqrt{2mV_0}}{\hbar}$

$$(139) \qquad \sigma = 4\pi a^2 \left(\frac{\tan k_{10} a}{k_{10} a} - 1 \right)^2$$



s-wave scattering resonances

$\sigma \to \infty$

At the resonances the s-wave scattering approximation for the total cross section is no longer good!

- resonances: $\qquad k_1 a = (2n+1)\frac{\pi}{2}$

boundary condition (136) $\Rightarrow$

$$0 = \cot(ka + \delta_0)$$

since $ka \ll 1 \quad \Rightarrow \quad \cot \delta_0 = 0 \quad$ or $\cos \delta_0 = 0$

$\sin \delta_0 \simeq 1$

thus

(140) $$\boxed{\frac{d\sigma}{d\Omega} = \frac{1}{k^2}\sin^2\delta_0 \cong \frac{1}{k^2}}$$ unitarity limit

and

(141) $$\boxed{\sigma = \frac{4\pi}{k^2}}$$

▶ What is the origin of the S-wave resonances?

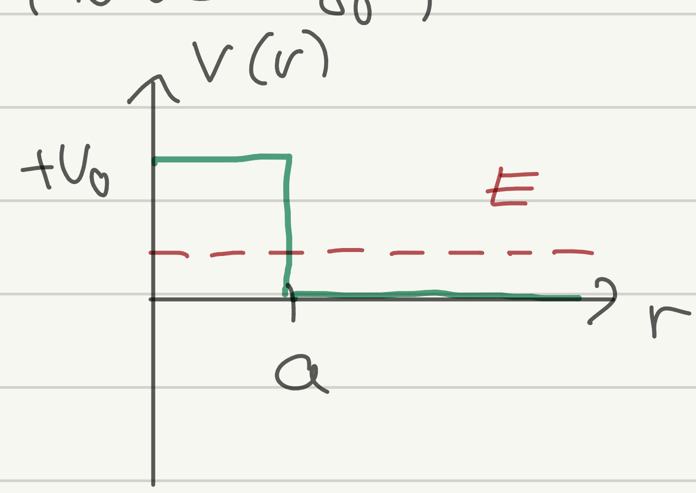
Answer: QM I $\rightarrow$ bound states for spherical well potential

at $k_1 a = (2n+1)\frac{\pi}{2}$ there is a bound state with energy

(142) $$\boxed{E_n \rightarrow 0}$$

Example 2: scattering off a repulsive spherical well (low energy)

(143) $$V(r) = \begin{cases} +V_0 & r < a \\ 0 & r > a \end{cases}$$



$V_0, a > 0$

here $u_1 = A\sinh(\varkappa r)$ $\quad \frac{\hbar^2\varkappa^2}{2m} = V_0 - E > 0$

analogous procedure as for example 1 ... $\Rightarrow$

(144) $$\sigma = 4\pi a^2 \left(\frac{\tanh \varkappa a}{\varkappa a} - 1 \right)^2$$

no resonances! for $V_0 \to \infty$: $\sigma = 4\pi a^2$

III.4 Two-particle scattering of identical particles

The interaction between particles leads to two-particle scattering events. As in classical mechanics we can reduce the scattering of two particles with an interaction potential of the form

(145) $$\boxed{V(\vec{r}_1, \vec{r}_2) = V(\vec{r}_1 - \vec{r}_2) = V(\vec{r})}$$

to an effective scattering problem of a single quantum particle. There is however one difference:

identical quantum particles $\equiv$ indistinguishable

$\Rightarrow$ Bosons $\quad \phi(\vec{r}_1, \vec{r}_2) = \phi(\vec{r}_2, \vec{r}_1)$

Fermions $\quad \phi(\vec{r}_1, \vec{r}_2) = -\phi(\vec{r}_2, \vec{r}_1)$

for potentials of type (145) we can solve the two-particle Schrödinger equation by introducing

$$(146) \quad \vec{r} = \vec{r}_1 - \vec{r}_2 \qquad \text{relative coordinate}$$

$$\vec{R} = \frac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2} \qquad \text{center-of-mass coordinate}$$

center-of-mass momentum is conserved (no external potential)

$$(147) \quad \phi(\vec{R}, \vec{r}) = \begin{cases} \phi(\vec{R}, -\vec{r}) & \text{bosons} \\ -\phi(\vec{R}, -\vec{r}) & \text{fermions} \end{cases}$$

$$\left(\frac{\hbar^2}{2\mu} \Delta_{\vec{r}} + V(\vec{r}) \right) \phi(\vec{R}, \vec{r}) = E - E_{com}$$

Due to the symmetry requirement (147) the partial-wave decomposition (121)

$$\varphi_k(r, \vartheta) = \sum_{\ell=0}^{\infty} C_\ell \frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)}{kr} P_\ell(\cos\vartheta)$$

where k is the relative momentum

$$(148) \quad k = |\vec{k}| = \left| \frac{1}{2} (\vec{k}_1 - \vec{k}_2) \right| \qquad E = \frac{\hbar^2 k^2}{2\mu}$$

has to be modified

$$\vec{r} \to -\vec{r} \quad \hat{=} \quad \cos\vartheta \to -\cos\vartheta$$

using $\qquad P_\ell(\cos\vartheta) = (-1)^\ell P_\ell(-\cos\vartheta)$

it follows

(148) $$\boxed{\begin{array}{l} C_{2\ell+1} \equiv 0 \text{ for bosons} \\ C_{2\ell} \equiv 0 \text{ for fermions} \end{array}}$$

i.e. there is no s-wave scattering for identical fermions

Bosons:

(149) $$\boxed{\varphi_k(r,\vartheta) = \sum_{n=0}^{\infty} C_{2n} \frac{\sin(kr - n\pi + \delta_{2n})}{kr} P_{2n}(\cos\vartheta)}$$

Fermions:

(150) $$\boxed{\phi_k(r,\vartheta) = \sum_{n=0}^{\infty} C_{2n+1} \frac{\sin(kr - \frac{2n+1}{2}\pi + \delta_{2n+1})}{kr} P_{2n+1}(\cos\vartheta)}$$

A consequence of the absence of s-wave scattering for identical fermions is that a gas of (spin polarized!) fermions has no scattering interactions at low temperatures.