Introduction to Scattering Theory

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Outline

Monday

- Stationary scattering states and elastic-scattering cross section
- Partial-wave expansion and notion of phase shift
- PM : Exercise session on phase shifts
- 2 Tuesday
 - Low- and high-energy behaviour of phase shift
 - Effective-range expansion
 - Notion of resonance
- Wednesday
 - S Matrix
 - Coulomb scattering



2 Notion of cross section

- Definition
- Theoretical framework
- Stationary Scattering States
- Theoretical scattering cross section

Partial-wave expansion and phase shift

- Partial-wave expansion
- Phase shift
- Scattering cross section

Quantum Collisions

Quantum collisions used to

• study the interaction between particles/nuclei/atoms...

(see Hans-Werner Hammer & Kai Hebeler's classes)

• analyse the structure of particles/nuclei/atoms...

(see Sonia Bacca & Daniel Phillips' classes)

measure reaction rates of particular interest

(stars, nuclear reactors, production of radioactive isotopes...) Measurement scheme : $\hfill \Omega$



Reaction types

Various reactions can happen :

- $a + b \rightarrow a + b$ (elastic scattering; this series of lectures)
- (inelastic scattering) $\rightarrow a + b^*$

Examples :

Energy conservation

Total energy is conserved : $m_a c^2 + m_b c^2$ + incident kinetic energy = mass of products c^2 + kinetic energy

The *Q* value is the energy "produced" by the reaction

$$m_a c^2 + m_b c^2 = \text{mass of products } c^2 + Q$$

 $\Leftrightarrow Q = m_a c^2 + m_b c^2 - \text{mass of products } c^2$

Q > 0: exoenergetic, always (energetically) possible Q < 0: endoenergetic, requires a minimal incident kinetic energy A channel can be open if the incident kinetic energy > -Qotherwise the channel is closed

The elastic channel is always open (Q = 0)



For an incident flux F_i on N particles in the target, the number Δn of events detected in direction $\Omega = (\theta, \varphi)$ per unit time within the solid angle $\Delta \Omega$ is proportional to F_i and N:

$$\Delta n = F_i N \Delta \sigma$$

The factor of proportionality σ is the cross section $[\Delta\sigma] = \text{surface}$; unit : barn 1 b = 10^{-24}cm^2 The differential cross section

$$\frac{d\sigma}{d\Omega} = \lim_{\Delta\Omega \to 0} \frac{\Delta\sigma}{\Delta\Omega} = \frac{\Delta n}{F_i N \Delta\Omega}$$

Taking Z as the beam axis, $d\sigma/d\Omega$ depends only on θ by symmetry

Theoretical framework

Let us consider particles *a* and *b* of mass m_a and m_b interacting through potential $V(\mathbf{r})$, where $\mathbf{r} = \mathbf{r}_a - \mathbf{r}_b$ is the *a*-*b* relative coordinate

The Hamiltonian reads

$$\mathcal{H} = T_a + T_b + V(\mathbf{r}),$$

where

$$T_a = \frac{p_a^2}{2m_a} = -\frac{\hbar^2 \Delta_{r_a}}{2m_a}$$
$$T_b = \frac{p_b^2}{2m_b} = -\frac{\hbar^2 \Delta_{r_b}}{2m_b}$$

Change to cm and *a-b* relative motion

The coordinate change

$$\boldsymbol{R}_{cm} = (m_a \boldsymbol{r}_a + m_b \boldsymbol{r}_b)/M$$
$$\boldsymbol{r} = \boldsymbol{r}_a - \boldsymbol{r}_b$$

with $M = m_a + m_b$, the total mass, leads to

$$\mathcal{H} = T_{\rm cm} + T_r + V(\mathbf{r}),$$

where
$$T_{\rm cm} = \frac{P_{\rm cm}^2}{2M} = -\frac{\hbar^2 \Delta_{R_{\rm cm}}}{2M}$$
$$T_r = \frac{p^2}{2\mu} = -\frac{\hbar^2 \Delta_r}{2\mu},$$

with $P_{cm} = p_a + p_b$, $p = (m_b p_a - m_a p_b)/M = \mu v$, and $\mu = m_a m_b/M$ the reduced mass of *a* and *b*

 \mathcal{H} is then the sum of two Hamiltonians : $H_{cm}(\mathbf{R}_{cm}) + H(\mathbf{r})$ Hence the two-body wave function factorises

$$\Psi_{\text{tot}}(\boldsymbol{r}_a, \boldsymbol{r}_b) = \Psi_{cm}(\boldsymbol{R}_{cm}) \ \Psi(\boldsymbol{r})$$



cm motion

The cm wave function is solution of

$$H_{cm} \Psi_{cm}(\boldsymbol{R}_{cm}) = E_{cm} \Psi_{cm}(\boldsymbol{R}_{cm}),$$

where
$$H_{cm} = \frac{P_{cm}^2}{2M}$$

is the Hamiltonian of a free particle of mass MThe cm motion is described by a plane wave

$$\Psi_{\boldsymbol{K}_{cm}}(\boldsymbol{R}_{cm}) = (2\pi)^{-3/2} e^{i \boldsymbol{K}_{cm} \cdot \boldsymbol{R}_{cm}}$$

with $E_{cm} = \hbar^2 K_{cm}^2 / 2M$

The factor $(2\pi)^{-3/2}$ is chosen such that

$$\langle \Psi_{\boldsymbol{K'}_{cm}} | \Psi_{\boldsymbol{K}_{cm}} \rangle = \delta(\boldsymbol{K}_{cm} - \boldsymbol{K'}_{cm})$$

Stationary Scattering States

The Hamiltonian of the *a*-*b* relative motion reads

$$H = T_r + V(\mathbf{r})$$

 $H = T_r + V(\mathbf{r}) \qquad \text{when} \quad T_{h=} - \frac{\hbar^2 \Delta_h}{2\mu}$ This is the Hamiltonian for a virtual particle of mass $\mu = \frac{m_e m_b^2}{m_e + m_b^2}$ evolving within the external potential well V

A stationary scattering state $\Psi_{k}(r)$ is solution of

$$H \Psi_{k} = E \Psi_{k}$$

where $E = \hbar^2 k^2 / 2\mu$ with the asymptotic behaviour

$$\Psi_{k\hat{\boldsymbol{z}}}(\boldsymbol{r}) \underset{r \to \infty}{\longrightarrow} (2\pi)^{-3/2} \left[e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r} \right],$$

with \hat{z} chosen as the beam axis f_k is the scattering amplitude

Physical interpretation

To interpret the stationary scattering state

$$\Psi_{k\hat{\boldsymbol{z}}}(\boldsymbol{r}) \underset{r \to \infty}{\longrightarrow} (2\pi)^{-3/2} \left[e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r} \right],$$

let us recall the probability current

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{1}{\mu} \mathfrak{R}[\Psi^*(\boldsymbol{r}) \, \boldsymbol{p} \, \Psi(\boldsymbol{r})]$$





Physical interpretation

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$$\boldsymbol{j}(\boldsymbol{r}) = \frac{1}{\mu} \mathfrak{R}[\Psi^*(\boldsymbol{r}) \, \boldsymbol{p} \, \Psi(\boldsymbol{r})]$$

The plane wave describes the incoming current

$$\mathbf{j}_i(\mathbf{r}) = (2\pi)^{-3} \frac{\hbar k}{\mu} \mathbf{\hat{z}} = (2\pi)^{-3} v \mathbf{\hat{z}}$$

where v is the *a*-*b* relative velocity

The spherical wave $f_k(\theta) \frac{e^{ikr}}{r}$ describes the scattered current

$$\boldsymbol{j}_{s}(\boldsymbol{r}) = (2\pi)^{-3} |\boldsymbol{v}| |f_{k}(\theta)|^{2} \frac{1}{r^{2}} \boldsymbol{\hat{r}} + O\left(\frac{1}{r^{3}}\right)$$

is purely radial at $R \to \infty$; directed outwards; $\propto v$ but varies with θ

Physical interpretation



Incoming wave :

Scattered wave :

$$e^{ikz} \rightarrow \boldsymbol{j}_i(\boldsymbol{r}) \propto \boldsymbol{v} \ \boldsymbol{\hat{z}}$$

$$f_k(\theta) \frac{e^{ikr}}{r} \rightarrow \boldsymbol{j}_s(\boldsymbol{r}) \propto v |f_k(\theta)|^2 \frac{1}{r^2} \boldsymbol{\hat{r}}$$

Theoretical scattering cross section

We can assume the incoming flux

 $F_i = C j_i$

The scattered flux in direction Ω is then

$$F_s(\Omega) = C \ j_s(\Omega)$$

For one scattering nucleus,

the number of events per unit time detected in direction Ω reads

$$\Delta m_{2} F_{i} \bigwedge_{i} \Delta \nabla \quad dn = F_{s}(\Omega) \, dS = C \, j_{s}(\Omega) \, r^{2} d\Omega$$

$$\Rightarrow \frac{d\sigma}{d\Omega} = \frac{dn}{F_{i} \, d\Omega}$$

$$\Rightarrow \frac{d\sigma}{f_{i}} = \frac{r^{2} j_{s}(\Omega)}{j_{i}}$$

$$= |f_{k}(\theta)|^{2}$$

The scattering amplitude f_k contains all information about V

Partial-wave expansion

If the potential does not depend on Ω , i.e. V(r),

$$[H, L^2] = 0$$

 $[H, L_Z] = 0$

the angular motion is described by spherical harmonics

$$\Psi(\boldsymbol{r}) = \frac{1}{r} \sum_{l,m} u_{kl}(r) Y_l^m(\Omega),$$

where u_{kl} is solution of the radial equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2}V(r) + k^2\right)u_{kl}(r) = 0$$

with $\frac{\hbar^2 k^2}{2\mu} = E$

Free wave

Let's start with no interaction : $V(r) = 0 \quad \forall r$ In that case u_{kl} is solution of

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right)u_{kl}(r) = 0$$

If we pose $u_{kl}(r) = x f_l(x)$, with x = kr, the equation becomes

$$\left(\frac{d^2}{dx^2} + \frac{2}{x}\frac{d}{dx} + 1 - \frac{l(l+1)}{x^2}\right)f_l(x) = 0$$

which is a spherical Bessel equation (aka Helmholtz equation) whose solutions are the spherical Bessel functions j_l and n_l n_l is sometimes called the spherical Neumann function

Spherical Bessel functions

$$j_{l}(x) = (-x)^{l} \left(\frac{1}{x}\frac{d}{dx}\right)^{l} \frac{\sin x}{x} \qquad n_{l}(x) = (-x)^{l} \left(\frac{1}{x}\frac{d}{dx}\right)^{l} \frac{\cos x}{x}$$

$$j_{0}(x) = \frac{\sin x}{x} \qquad n_{0}(x) = \frac{\cos x}{x}$$

$$j_{1}(x) = \frac{\sin x}{x^{2}} - \frac{\cos x}{x} \qquad n_{1}(x) = \frac{\cos x}{x^{2}} + \frac{\sin x}{x}$$

$$j_{l}(x) \xrightarrow[x \to 0]{} \frac{x^{l}}{(2l+1)!!} \qquad n_{l}(x) \xrightarrow[x \to 0]{} \frac{(2l-1)!!}{x^{l+1}}$$

$$j_{l}(x) \xrightarrow[x \to \infty]{} \frac{1}{x}\sin(x-l\frac{\pi}{2}) \qquad n_{l}(x) \xrightarrow[x \to \infty]{} \frac{1}{x}\cos(x-l\frac{\pi}{2})$$

Recurrence relations : for $f_l = j_l$ or n_l ,

$$\begin{aligned} xf'_{l}(x) &= xf_{l-1}(x) - (l+1)f_{l}(x) \\ xf'_{l}(x) &= lf_{l}(x) - xf_{l+1}(x) \\ (2l+1)x^{-1}f_{l}(x) &= f_{l+1}(x) + f_{l-1}(x) \end{aligned}$$

Plane waves and spherical Bessel functions When V(r) = 0 $\forall r$, the plane wave e^{ikz} (so with $f_k(\theta) = 0$) is also a solution of the Schrödinger equation, so

$$e^{ikz} = \sum_{l=0}^{\infty} \left[a_l \ j_l(kr) + b_l \ n_l(kr) \right] Y_l^0(\Omega)$$
$$b_l = 0 \quad \forall l \text{ since } n_l(kr) \xrightarrow[r \to 0]{} \frac{(2l-1)!!}{(kr)^{l+1}} \checkmark$$

For a_l , one gets

$$a_l = i^l \sqrt{4\pi(2l+1)}$$

and

$$e^{ikz} = \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} j_l(kr) Y_l^0(\Omega)$$

$$\xrightarrow[r \to \infty]{} \sum_{l=0}^{\infty} i^l \sqrt{4\pi(2l+1)} \frac{1}{kr} \sin(kr - l\pi/2) Y_l^0(\Omega)$$

Distorted wave

Switching on the *a*-*b* interaction ($V \neq 0$), we have to solve the radial equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2}V(r) + k^2\right)u_{kl}(r) = 0$$

with $\frac{\hbar^2 k^2}{2\mu} = E$ But for a "few" cases (see exercises this afternoon) it is done numerically (see exercises new week with N. Barnea and S. Bacca)

To compute the cross section from the solution u_{kl} we need the scattering amplitude $f_k(\theta)$ which is deduced from the asymptotics of the wave function

If we assume
$$r^2 V(r) \xrightarrow[r \to \infty]{} 0$$
, $u_{kl}(r) \xrightarrow[r \to \infty]{} u_{kl}^{as}(r)$, which is solution of

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right) u_{kl}^{as}(r) = 0$$

Phase shift δ_l

The solutions of

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2\right)u_{kl}^{\rm as}(r) = 0$$

are once again spherical Bessel functions

$$u_{kl}^{as}(r) = a_l kr j_l(kr) + b_l kr n_l(kr)$$

$$\xrightarrow[r \to \infty]{} a_l \sin(kr - l\pi/2) + b_l \cos(kr - l\pi/2)$$

Posing $a_l = c_l \cos \delta_l$ and $b_l = c_l \sin \delta_l$

$$u_{kl}^{as}(r) \xrightarrow[r \to \infty]{} c_l \sin(kr - l\pi/2 + \delta_l)$$

 c_l is just a normalisation factor

 δ_l is the phaseshift : it contains all information on the influence of V

Phase shift : Physical interpretation The asymptotics of the distorted wave $(V \neq 0)$

$$u_{kl}^{as}(r) \underset{r \to \infty}{\longrightarrow} c_l \sin(kr - l\pi/2 + \delta_l)$$

is phase shifted compared to the plane wave (V = o)

$$a_l kr j_{kl}(r) \underset{r \to \infty}{\longrightarrow} a_l \sin(kr - l\pi/2)$$



Phase shift

Phase shift : Physical interpretation The asymptotics of the distorted wave

$$u_{kl}^{as}(r) \underset{r \to \infty}{\longrightarrow} c_l \sin(kr - l\pi/2 + \delta_l)$$

is phase shifted compared to the plane wave

$$a_l kr j_{kl}(r) \xrightarrow[r \to \infty]{} a_l \sin(kr - l\pi/2)$$

- $V(r) < 0 \quad \forall r \implies \delta_l > 0$: wave attracted by the field the colliding particles tend to stick together
- V(r) > 0 $\forall r \Rightarrow \delta_l < 0$: wave repulsed by the field the colliding particles repulse each other

(see exercises this afternoon)

Scattering matrix S₁

Another way of seeing this is to interpret

$$u_{kl}^{as}(r) \xrightarrow[r \to \infty]{} c_l \sin(kr - l\pi/2 + \delta_l)$$

in terms of incoming and outgoing (spherical) waves :

$$u_{kl}(r) \xrightarrow[r\to\infty]{} i c_l \frac{e^{-i\delta_l}}{2} \left[e^{-i(kr-l\pi/2)} - S_l e^{i(kr-l\pi/2)} \right]$$

where

$$S_l = e^{2i\delta_l}$$

is the scattering matrix or S matrix

The outgoing wave is shifted from the incoming wave by $2\delta_l$ due to the effect of $V \Rightarrow$ used to compute the scattering amplitude f_k

Scattering amplitude

The scattering wave function can be expanded in partial waves

$$(2\pi)^{3/2} \Psi_{k\hat{z}}(\mathbf{r}) = \frac{1}{kr} \sum_{l=0}^{\infty} u_{kr}(r) Y_{l}^{0}(\Omega)$$

$$\xrightarrow{r \to \infty} e^{ikz} + f_{k}(\theta) \frac{e^{ikr}}{r}$$

Since $e^{ikz} \xrightarrow{r \to \infty} \sum_{l=0}^{\infty} i^{l} \sqrt{4\pi(2l+1)} \frac{i}{2kr} \left[e^{-i(kr-l\pi/2)} - e^{i(kr-l\pi/2)} \right] Y_{l}^{0}(\Omega)$
and $u_{kl} \xrightarrow{r \to \infty} i c_{l} \frac{e^{-i\delta_{l}}}{2} \left[e^{-i(kr-l\pi/2)} - S_{l} e^{i(kr-l\pi/2)} \right]$

comparing the incoming waves we obtain $c_l = i^l \sqrt{4\pi(2l+1)} e^{i\delta_l}$ and deduce the scattering amplitude from $S_{I} = e^{2i\delta_{I}}$

$$f_k(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)} (S_l - 1) Y_l^0(\Omega) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) (S_l - 1) P_l(\cos\theta)$$

Scattering cross section $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2$ $= \left|\frac{1}{2ik}\sum_{l=0}^{\infty} (2l+1)(S_l-1)P_l(\cos\theta)\right|^2$

After integration over Ω the total scattering cross section reads





Contribution of partial waves

Each partial wave contributes to σ but with variable importance



At very low *E*, only l = 0 contributes and $\sigma = \frac{4\pi}{k^2} \sin^2 \delta_0$

At large *E* many partial waves must be included to reach convergence (\Rightarrow low-energy method)

How to compute δ_l ?

For short-range potentials, space can be divided in two regions :

• External one, where $V(r) \approx 0$ $\forall r > r_0$, where $u_{kl}(r)$ is

$$u_{kl}^{as}(r) = c_l \left[\cos \delta_l \, kr \, j_l(kr) + \sin \delta_l \, kr \, n_l(kr) \right] \underset{r \to \infty}{\longrightarrow} c_l \sin(kr - l\pi/2 + \delta_l)$$

• Internal one $(r < r_0)$, where V is non-negligible and where we have to solve the radial equation

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2}V(r) + k^2\right)u_{kl}^{\text{int}}(r) = 0$$

e.g. numerically (see exercises next week with N. Barnea and S. Bacca) At the boundary

$$u_{kl}^{\text{int}}(r_0) = u_{kl}^{\text{as}}(r_0) \text{ and } u_{kl}^{\text{int}'}(r_0) = u_{kl}^{\text{as}'}(r_0)$$

or $\frac{u_{kl}^{\text{int}'}}{u_{kl}^{\text{int}'}}\Big|_{r_0} = \frac{u_{kl}^{\text{as}'}}{u_{kl}^{\text{as}}}\Big|_{r_0} = \frac{k\cos(kr_0 - l\pi/2 + \delta_l)}{\sin(kr_0 - l\pi/2 + \delta_l)},$

which gives access to the phase shift δ_l (see exercises this afternoon)

How to infer δ_l from data?

Because the elastic-scattering cross section is a function of δ_l

$$\frac{d\sigma}{d\Omega} = \left|\frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(S_l-1)P_l(\cos\theta)\right|^2,$$

experimental phase shifts can be obtained from data

A development of the differential cross section in Legendre polynomials P_l provides δ_l "experimentally"

(see exercises this afternoon)

Example : p-n phaseshifts Notation : ${}^{2S+1}L_{I}$



[Navarro Pérez, Amaro, Ruiz Arriola, PLB 724 138 (2013)] Data used to fit the various terms of V_{NN} (see lectures of Kai Hebeler)

Summary

- Collisions used to study interaction and structure of "particles"
- Notion of cross section used to characterise a process in quantum collision theory

$$\frac{d\sigma}{d\Omega} = \lim_{\Delta\Omega \to 0} \frac{\Delta n}{F_i N \Delta \Omega}$$

• Computing stationary scattering state

$$\Psi_{k\hat{\boldsymbol{\zeta}}}(\boldsymbol{r}) \underset{r \to \infty}{\longrightarrow} (2\pi)^{-3/2} \left[e^{ikz} + f_k(\theta) \frac{e^{ikr}}{r} \right],$$

gives the scattering cross section

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

Summary (2)

• In partial-wave expansion, defining phaseshifts

$$u_{kl}^{as}(r) \xrightarrow[r \to \infty]{} c_l \sin(kr - l\pi/2 + \delta_l)$$

the scattering cross section reads

$$\frac{d\sigma}{d\Omega} = \left| \frac{1}{k} \sum_{l=0}^{\infty} (2l+1)(S_l-1)P_l(\cos\theta) \right|^2$$

• Phase shifts δ_l obtained by solving the radial equation for $r < r_0$

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - \frac{2\mu}{\hbar^2}V(r) + k^2\right)u_{kl}^{\text{int}}(r) = 0$$

and matching the solution with the external one u_{kl}^{as} :

$$\frac{u_{kl}^{\text{int}}}{u_{kl}^{\text{int}}}\bigg|_{r_0} = \frac{u_{kl}^{\text{as}\prime}}{u_{kl}^{\text{as}}}\bigg|_{r_0}$$

Bibliography

The following books are good references for more details on low-energy nuclear-reaction theory :

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