Introduction to Scattering Theory III

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Relation between phase shift and potential

We consider two scattering potentials V and $\bar{V}$

$$\sin(\delta_l - \bar{\delta}_l) = -\frac{2\mu}{\hbar^2} k \int_0^\infty \bar{u}_{kl}(r) \left[V(r) - \bar{V}(r) \right] u_{kl}(r) \, dr$$

This provides two pieces of information :

1. Change in δ_l goes opposite to the change in V :
   $V(r) > \bar{V}(r) \; \forall r \Rightarrow \delta_l(k) < \bar{\delta}_l(k) \; \forall k$
   - repulsive potential ($V(r) > 0 \; \forall r$) $\Rightarrow \delta_l(k) < 0 \; \forall k$
   - attractive potential ($V(r) < 0 \; \forall r$) $\Rightarrow \delta_l(k) > 0 \; \forall k$
2. Choosing $\bar{V} = 0$, we obtain an integral expression for δ_l :

$$\sin \delta_l = -\frac{2\mu}{\hbar^2} k \int_0^\infty j_{kl}(kr) V(r) R_{kl}(r) \, r^2 dr$$

[with $R_{kl}(r) = \frac{1}{r} u_{kl}(r)$]

Phase shift at low-energy

$$\tan \delta_l \quad \underset{k \to 0}{\longrightarrow} \quad \frac{(kr_0)^{2l+1}}{(2l+1)!!(2l-1)!!} \frac{l - r_0\gamma_l}{(l+1) + r_0\gamma_l}$$

(unless $(l+1) + r_0\gamma_l = 0$)

In the s wave, the scattering length

$$a \quad = \quad -\lim_{k \to 0} \frac{\tan \delta_0}{k}$$

At very low energy,
only the s wave contributes to the scattering cross section
and $\frac{d\sigma}{d\Omega} \underset{k \to 0}{\longrightarrow} a^2$: the differential cross section is isotropic

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

S wave $(\ell = 0)$ $\quad k \to 0 \quad \left(u_{k\ell} \longrightarrow u^0\right)$

$$\left[\frac{d^2}{dr^2} - \frac{2\mu}{\hbar^2} V(r)\right] u^0(r) = 0$$

$r > r_0$

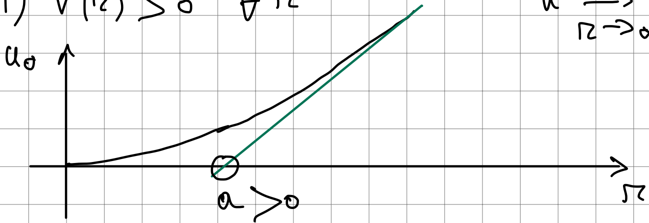
$$u^{0\,\prime\prime}(r) = 0 \quad \Longrightarrow \quad u^0(r) = Br + C$$

$$u^0(r) \xrightarrow[k \to 0]{} \frac{1}{k} \sin(kr + \underbrace{\delta_0}_{\to -ak})$$

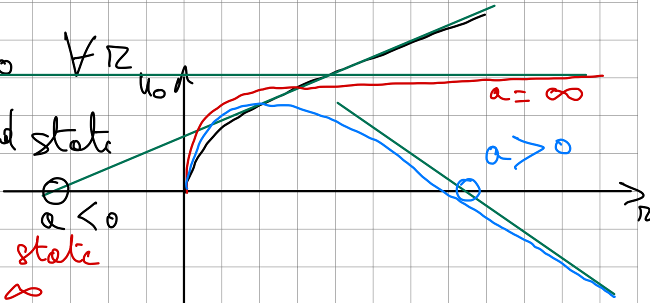
$$\xrightarrow[k \to 0]{} (r - a)$$

1) $V(r) > 0 \quad \forall r$

$$u^0 \xrightarrow[r \to \infty]{} (r - a)$$



2) $V(r) < 0 \quad \forall r$



- no bound state
- virtual state
  $a = \infty$
- bound state
  $a > 0$

Effective-range expansion

In partial wave l, the function $k^{2l+1} \cot \delta_l$ is analytic in E, i.e. in k^2.

It can be expanded in powers of E (see Hans' 2nd lecture)

In the s wave, the first coefficient is the scattering length a

$$k \cot \delta_0 = -\frac{1}{a} + \frac{r_e}{2} k^2 + \frac{P}{4} k^4 + \ldots$$

where

- r_e is the effective range
- P is the shape parameter
- …

For $l > 0$

$$k^{2l+1} \cot \delta_l = -\frac{1}{a_l} + \frac{r_l}{2} k^2 + \frac{P_l}{4} k^4 + \ldots$$

S wave ($\ell = 0$) $\quad u_1, u_2 \qquad u_i(r) \xrightarrow[r\to\infty]{} \dfrac{\sin(k_i r + \delta_0^i)}{\sin(\delta_0^i)}$

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{2\mu}{\hbar^2} V(r)\right] u_i(r) = 0$$

$$\frac{d}{dr}\left[u_1 u_2' - u_2 u_1'\right] = \cancel{u_1' u_2'} + u_1 u_2'' - \cancel{u_2' u_1'} - u_2 u_1''$$

$$= \left[-k_2^2 + \cancel{\frac{2\mu}{\hbar^2} V(r)}\right] u_1 u_2$$

$$- \left[-k_1^2 + \cancel{\frac{2\mu}{\hbar^2} V(r)}\right] u_2 u_1$$

$$= (k_1^2 - k_2^2)\, u_1 u_2$$

$v_1, v_2 \qquad v_i = \dfrac{\sin(k_i r + \delta_0^i)}{\sin \delta_0^i} \xrightarrow[r\to 0]{} 1$

$$\left[\frac{d^2}{dr^2} + k_i^2\right] v_i(r) = 0 \qquad u_i(r) \xrightarrow[r\to\infty]{} v_i(r)$$

$$\int_0^\infty \frac{d}{dr}\left[u_1 u_2' - u_2 u_1' - v_1 v_2' + v_1' v_2\right] dr$$

$$= \left(k_1^2 - k_2^2\right) \int_0^\infty \left[u_1(r) u_2(r) - v_1(r) v_2(r)\right] dr$$

$$= \left[u_1 u_2' - u_2 u_1' - v_1 v_2' + v_1' v_2\right]_0^\infty$$

$$\underset{u_i \xrightarrow[r\to\infty]{} v_i}{=} 0 \quad - 0 + 0 - v_1(0)\, v_2'(0) + v_1'(0)\, v_2'(0)$$

$$= -1 \cdot k_2 \cot \delta_0^2 + k_1 \cot \delta_0^1 \cdot 1$$

$$= k_1 \cot \delta_0^1 - k_2 \cot \delta_0^2$$

take the limit $k_2 \to 0$ posing $k_1 = k$

$$k \cot \delta_0 + \frac{1}{a} = k^2 \int_0^\infty \left[u_k(r) u_0(r) - v_k(r) v_0(r) \right] dr$$
$$= k^2 \int_0^{r_0} \left[u_k(r) u_0(r) - v_k(r) v_0(r) \right] dr$$

Since we have

$$k \cot \delta_0 = -\frac{1}{a} + \frac{r_e}{2} k^2 + \dots$$

We deduce

$$r_e = 2 \lim_{k \to 0} \int_0^{r_0} \left[u_k(r) u_0(r) - v_k(r) v_0(r) \right] dr$$
$$= 2 \int_0^{r_0} \left[u_0^2(r) - v_0^2(r) \right] dr$$

Relation with bound states

A similar development can be done using a bound state $(u^2 \rightarrow u^\kappa)$

So with the two solutions $(v^2 \rightarrow v^\kappa)$

$$\left[\frac{d^2}{dr^2} - \kappa^2 - \frac{2\mu}{\hbar^2}V(r)\right]u^\kappa(r) = 0$$

$$\left[\frac{d^2}{dr^2} - \kappa^2\right]v^\kappa(r) = 0, \qquad \text{where } -\frac{\hbar^2}{2\mu}\kappa^2 = E_0$$

Therefore

$$u^\kappa(0) = 0 \text{ and } u^\kappa(r) \underset{r\to\infty}{\longrightarrow} e^{-\kappa r}$$

$$v^\kappa(r) = e^{-\kappa r} \quad (v^\kappa(0) = 1)$$

For which we have (approximating u^κ and v^κ by u^0 and v^0)

$$k \cot\delta_0(k) + \kappa = \frac{1}{2}r_e(k^2 + \kappa^2)$$

$$\underset{k\to 0}{\longrightarrow} \quad -\frac{1}{a} = -\kappa + \frac{1}{2}r_e\kappa^2$$

Phase shift at high-energy

To study the phase shift at high energy, let us consider the integral expression of the phase shift

$$\sin\delta_l \approx -\frac{2\mu}{\hbar^2} k \int_0^\infty j_l^2(kr)\, V(r)\, r^2\, dr$$

assuming $R_{kl}(r) \approx j_l(kr)$ (first Born approximation)
Since $j_l(x) \underset{x\to\infty}{\longrightarrow} \frac{1}{x}\sin(x - l\pi/2)$ $\Rightarrow$ $j_l^2(kr) \underset{k\to\infty}{\longrightarrow} \frac{1}{k^2 r^2}\sin^2\left(kr - \frac{l\pi}{2}\right)$

$= \frac{1}{2k^2 r^2}\left[1 - \cos(2kr - l\pi)\right]$

$$\begin{aligned}
\sin\delta_l &\approx -\frac{\mu}{\hbar^2}\frac{1}{k}\int_0^\infty V(r)\, dr \\
&\underset{k\to\infty}{\longrightarrow} 0 \\
\Rightarrow \delta_l &\underset{k\to\infty}{\longrightarrow} 0 \;\; (+n\pi)
\end{aligned}$$

Imposing $\delta_l \underset{k\to\infty}{\longrightarrow} 0$ is similar to imposing $\delta_l = 0$ when $V = 0$

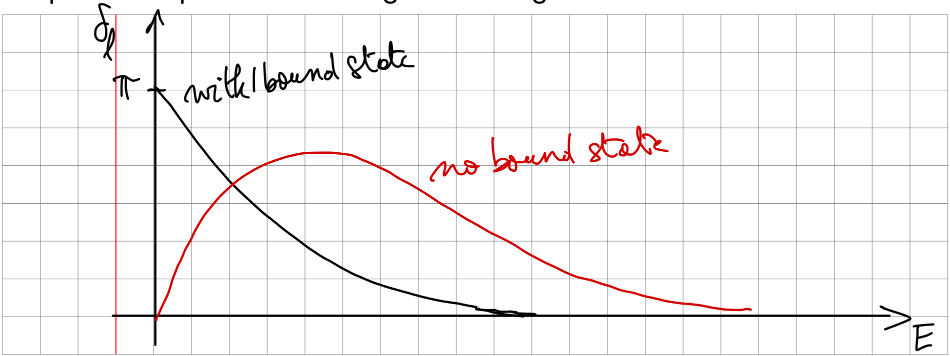
Levinson Theorem

That theorem relates the phase shift at $E = 0$ to that at $E \to \infty$.
It states that

$$\delta_l(0) - \delta(\infty) = N_l \pi,$$

where N_l is the number of bound states in the partial wave l

It relates the properties of the solutions of the radial Schrödinger equation at positive and negative energies.



Summary : Properties of phase shifts

- By convention

$$V(r) = 0 \ \ \forall r \quad \Rightarrow \quad \delta_l = 0 \ \ \forall E$$
$$\Leftrightarrow \delta_l \ \underset{k\to\infty}{\longrightarrow} \ 0$$

- δ_l is a continuous function of energy
  moreover $k^{2l+1} \cot \delta_l$ is analytical in E
- If $V(r) > \bar{V}(r) \ \forall r$, then $\delta_l < \bar{\delta}_l \ \forall E$
  $\Rightarrow$ if $V(r) < 0 \ \forall r$ (attractive), then $\delta_l > 0 \ \forall E$
  $\Rightarrow$ if $V(r) > 0 \ \forall r$ (repulsive), then $\delta_l < 0 \ \forall E$
- At low energy

$$\delta_l(k) - \delta_l(0) \sim k^{2l+1}$$

- Levinson Theorem :

$$\delta_l(0) - \delta(\infty) = N_l \, \pi,$$

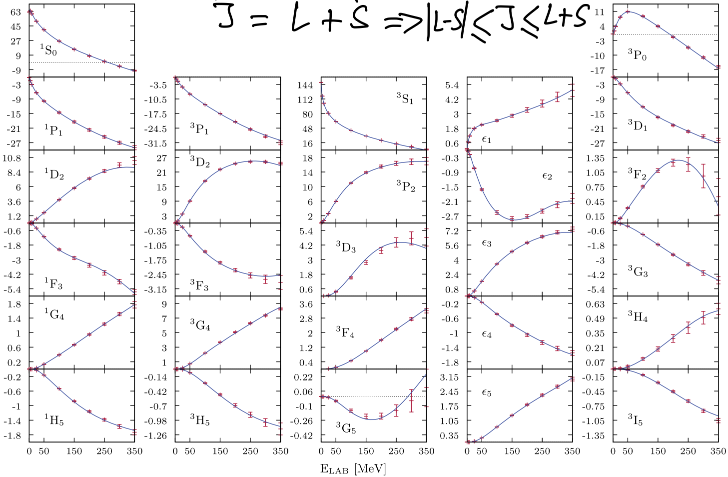
where N_l is the number of bound states in the partial wave l

Example : p-n phaseshifts

Notation : ${}^{2S+1}L_J$

$\vec{S} = \vec{S}_p + \vec{S}_n \Rightarrow S = 0$, or 1

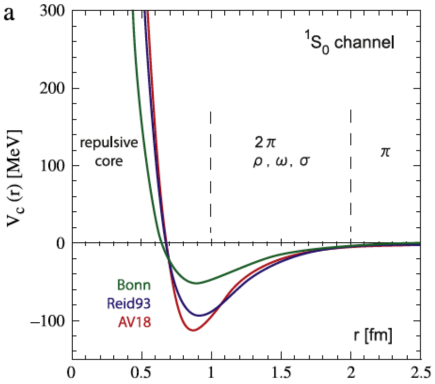
$\vec{J} = \vec{L} + \vec{S} \Rightarrow |L-S| \leq J \leq L+S$



[Navarro Pérez, Amaro, Ruiz Arriola, PLB 724 138 (2013)]

Data used to fit the various terms of V_{NN} (see lectures of Kai Hebeler)

Realistic V_{NN}



(see Kai's lecture)

Strongly repulsive core ⇒ negative phaseshifts

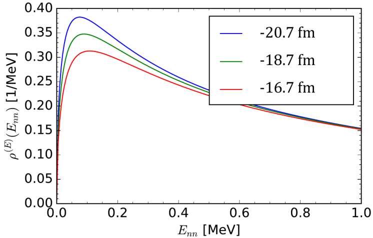
Short distaces ⇔ high energies

a_{nn}

a_{nn} is large and negative,
but discrepancy between experimental measurements

- $a_{\mathrm{nn}} = -18.7(6)$ fm (TUNL)
- $a_{\mathrm{nn}} = -16.2(3)$ fm (Bonn)
- $a_{\mathrm{pp}} = -17.3(4)$ fm

$^6\mathrm{He} + \mathrm{p} \to \alpha + \mathrm{n} + \mathrm{n} + \mathrm{p}$ will be measured at RIKEN (Japan)



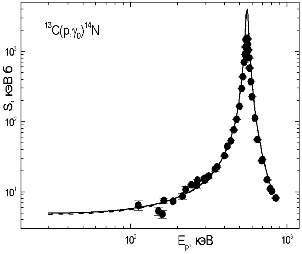
(from Hans' group)

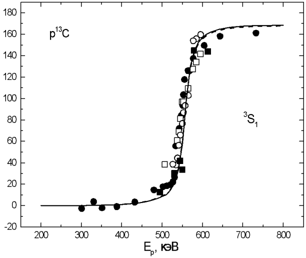
Energy spectrum will constrain a_{nn}

Notion of Resonance

Resonance $\equiv$

significant variation of a cross section on a short energy range





[Dubovichenko PAN 75, 173 (2012)]

In elastic scattering, contribution of partial wave l

$$\sigma_l = \frac{4\pi}{k^2}(2l+1)\sin^2\delta_l$$

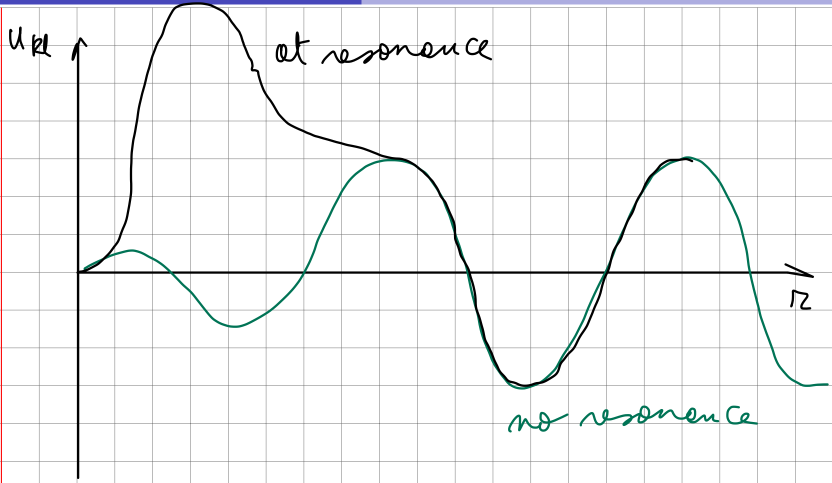
small if $\delta_l \sim n\pi \ (n \in \mathbb{Z})$

large if $\delta_l \sim \pi/2$

If δ_l goes quickly from 0 to $\pi \rightarrow$ rapid increase and decrease of σ_l

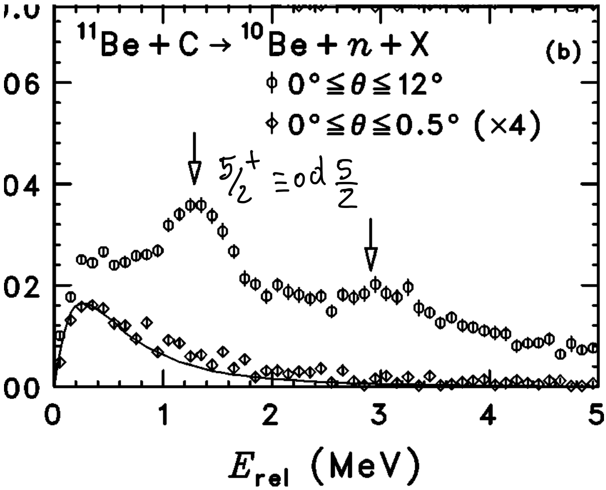
i.e. resonance structure

Definite $l \Rightarrow$ quantum numbers and parity similar to bound state


u_{kl}
at resonance
r
no resonance

Another example : nuclear breakup of ^{11}Be

$$^{11}\mathrm{Be} + \, ^{12}\mathrm{C} \rightarrow \, ^{10}\mathrm{Be} + \mathrm{n} + \, ^{12}\mathrm{C} \quad @ \; 67\mathrm{AMeV}$$



[Fukuda *et al.* PRC 70, 054606 (2004)]

Back to the S matrix

Let's rewrite the asymptotic expression

$$u_{kl}(r) \xrightarrow[r\to\infty]{} \frac{1}{2i}\left[f_l(k)\, e^{-i(kr-l\pi/2)} - f_l^*(k)\, e^{i(kr-l\pi/2)}\right] \in \mathbb{R}$$

in that case

$$S_l(k) = e^{2i\delta_l} = \frac{f_l^*(k)}{f_l(k)}$$

So far we have considered $k \in \mathbb{R}^+$ (since $E > 0$)
Now let's extend this to the complex plane

(f_l is continuous and analytic)

If $k_0 = k_R + ik_I$ is a zero of f_l : $f_l(k_0) = 0$

$$u_{k_0 l}(r) \xrightarrow[r\to\infty]{} e^{ik_R r} e^{-k_I r}$$

- if $k_R = 0$ and $k_I > 0$, it corresponds to a bound state
- if $k_R > 0$ and $k_I < 0$, it corresponds to a resonance

Poles of the S matrix

Since $S_l = \frac{f_l^*}{f_l}$, a zero of f corresponds to a pole of S_l

Close to that pole

$$\begin{aligned} S_l(k) &= e^{2i\phi}\frac{k-k_0^*}{k-k_0} \\ \text{or} \quad S_l(E) &= e^{2i\phi}\frac{E-E_0^*}{E-E_0} \\ \text{with} \quad E_0 &= \frac{\hbar^2}{2\mu}k_0^2 = E_r - i\Gamma/2 \end{aligned}$$

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

$$\delta_l = -\phi + \arctan\frac{\Gamma/2}{E_r - E}$$

When $\phi \ll 1$, $\delta(E_r) = \pi/2$, $\delta(E_r - \Gamma/2) = \pi/4$, $\delta(E_r + \Gamma/2) = 3\pi/4$

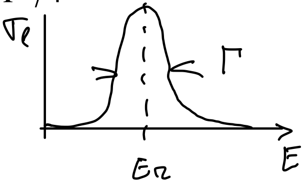
We also have

$$\left.\frac{d\delta_l}{dE}\right|_{E_r} = \frac{2}{\Gamma}$$

Breit-Wigner formula

The contribution of the l partial wave to the cross section

$$
\begin{aligned}
\sigma_l &= \frac{4\pi}{k^2}(2l+1)\frac{\tan^2\delta_l}{1+\tan^2\delta_l} \quad \left(= \sin^2\delta_l\right) \\
&= \frac{4\pi}{k^2}(2l+1)\frac{\Gamma^2/4}{(E_r-E)^2+\Gamma^2/4}
\end{aligned}
$$



This is the Breit-Wigner formula (Lorentzian)

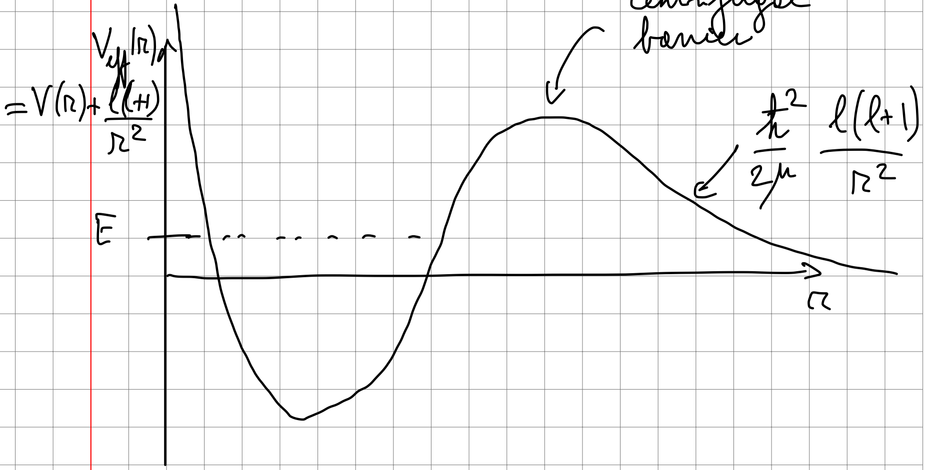
Since $\sigma_l(E_r-\Gamma/2)=\sigma_l(E_r+\Gamma/2)=\sigma_l(E_r)/2$

Γ is the full width at half maximum (FWHM)
Related to the lifetime of the resonance

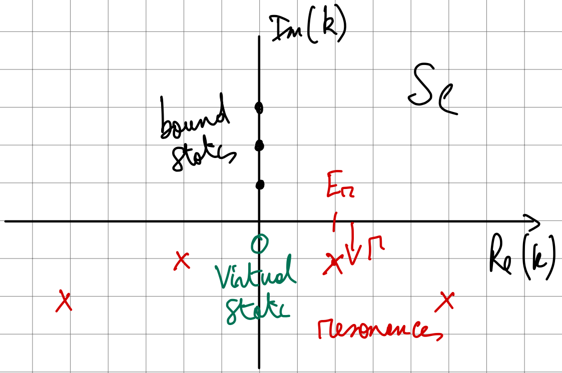
$$\tau = \frac{\hbar}{\Gamma}$$

When the non-resonant phase ϕ is not negligible
the shape can differ significantly from a simple Lorentzian

Interpretation of a resonance as a state in a potential pocket due to the centrifugal barrier.



Bound states, resonances, and virtual state seen as pole of the S matrix in the complex plane.



Coulomb scattering

We assumed $r^2 V(r) \underset{r\to\infty}{\longrightarrow} 0$, which excludes Coulomb $V_C(r) = \frac{Z_a Z_b e^2}{4\pi\epsilon_0 r}$

Coulomb requires special treatment, but similar results are obtained

Defining the Sommerfeld parameter $\eta = \frac{Z_a Z_b e^2}{4\pi\epsilon_0 \hbar v}$,

Schrödinger equation for a and b scattered by Coulomb reads

$$\left(\Delta - \frac{2\eta k}{r} + k^2\right)\Psi_C(\boldsymbol{r}) = 0,$$

which can be solved exactly and

$$\Psi_C(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} (2\pi)^{-3/2}\left(e^{i\left[kz+\eta\ln k(r-z)\right]} + f_C(\theta)\frac{e^{i\left[kr-\eta\ln 2kr\right]}}{r}\right),$$

with $f_C(\theta) = -\frac{\eta}{2k\sin^2(\theta/2)}e^{2i\left[\sigma_0-\eta\ln\sin(\theta/2)\right]}$ $\quad [\sigma_0 = \arg\Gamma(1+i\eta)]$

the Coulomb scattering amplitude

Rutherford cross section

The same analysis can be done defining $\boldsymbol{j}_i$ and $\boldsymbol{j}_s$ to define the Coulomb elastic scattering cross section or Rutherford cross section :

$$\begin{aligned}\frac{d\sigma_R}{d\Omega} &= |f_C(\theta)|^2 \\ &= \left(\frac{Z_a Z_b e^2}{4\pi\epsilon_0}\right)^2 \frac{1}{16E^2 \sin^4(\theta/2)}\end{aligned}$$

Note that it diverges at $\theta = 0$

Partial-wave analysis

We can again separate the angular from the radial part solution of

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

If additional (nuclear) term $r^2 V_N(r) \underset{r\to\infty}{\longrightarrow} 0$, $u_{kl}(r) \underset{r\to\infty}{\longrightarrow} u_{kl}^{\mathrm{as}}(r)$:

$$\begin{aligned} u_{kl}^{\mathrm{as}}(r) &= A\ F_l(\eta, kr) + B\ G_l(\eta, kr) \\ &\underset{r\to\infty}{\longrightarrow} A \sin(kr - l\pi/2 - \eta \ln kr + \sigma_l) \\ &\quad + B \cos(kr - l\pi/2 - \eta \ln kr + \sigma_l) \end{aligned}$$

where F_l and G_l are regular and irregular Coulomb functions
and $\sigma_l = \arg \Gamma(l + 1 + i\eta)$ is the Coulomb phaseshift

$$\Rightarrow u_{kl}^{\mathrm{as}}(r) \underset{r\to\infty}{\longrightarrow} C \sin(kr - l\pi/2 - \eta \ln kr + \sigma_l + \delta_l)$$

δ_l is an additional phaseshift,
which contains all information about the nuclear interaction V_N

(Additional) scattering amplitude

The stationary scattering states have now the asymptotic behaviour

$$\Psi(\boldsymbol{r}) \underset{r\to\infty}{\longrightarrow} \Psi_C(\boldsymbol{r}) + (2\pi)^{-3/2} f_{\text{add}}(\theta) \frac{e^{i(kr-\eta \ln kr)}}{r}$$

$$\text{with} \quad f_{\text{add}}(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) e^{2i\sigma_l} (e^{2i\delta_l} - 1) P_l(\cos\theta)$$

the additional scattering amplitude

The total scattering amplitude $f(\theta) = f_C(\theta) + f_{\text{add}}(\theta)$

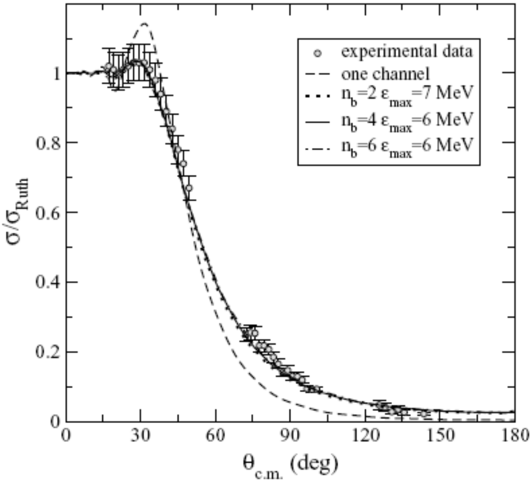
gives the elastic-scattering cross section

$$\frac{d\sigma}{d\Omega} = |f_C(\theta) + f_{\text{add}}(\theta)|^2$$

At forward angles ($\theta \ll 1$), $f_C \gg f_{\text{add}}$, and $d\sigma/d\Omega \approx d\sigma_R/d\Omega$

$\Rightarrow$ usually $(d\sigma/d\Omega)/(d\sigma_R/d\Omega)$ is plotted

Example : $^{6}\mathrm{He}$ + $^{64}\mathrm{Zn}$ @ 14MeV



[Rodrìguez-Gallardo *et al.* PRC 77, 064609 (2008)]

Bibliography

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

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