2.7 Partial-wave analysis

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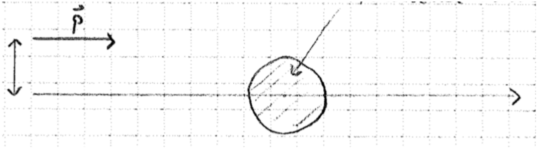
- Partial-wave decomposition:
  - based on an expansion of the wave function in angular-momentum eigenstates
  - particularly well suited for small energies
- classical picture:



- Only particles with $b \leq R$ are scattered.

  $\Rightarrow$ Only angular momenta $|\vec{\ell}| \leq R|\vec{p}|$ contribute to the cross section.

- Schrödinger equation with radially symmetric potential $V(\vec{r}) = V(r)$:

$$\left(-\frac{\hbar^2}{2\mu}\vec{\nabla}^2 + V(r)\right)\psi(\vec{r}) = E\psi(\vec{r})$$

- reminder: $\vec{\nabla}^2 = \Delta = \frac{1}{r}\frac{\partial^2}{\partial r^2} r - \frac{\vec{L}^2}{\hbar^2 r^2}$
  - orbital angular momentum: $\vec{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)$
  - eigenfunctions: $\vec{L}^2\, Y_\ell^m(\theta,\varphi) = \ell(\ell+1)\,\hbar^2\, Y_\ell^m(\theta,\varphi)$

➞ solutions of the Schrödinger eq. with well defined orbital angular momentum:

$$\psi_{\ell m}(\vec{r}) = R_\ell(r) Y_\ell^m(\theta,\varphi) \equiv \frac{u_\ell(r)}{r} Y_\ell^m(\theta,\varphi)$$

- equation for the radial part: $\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \underbrace{V(r) + \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}}_{V_{\text{eff}}(r)}\right)u_\ell(r) = E u_\ell(r)$

- Define: $U(r) = \frac{2\mu}{\hbar^2} V(r), \quad k^2 = \frac{2\mu}{\hbar^2} E \quad$ (as before)

$$\Rightarrow \boxed{\left(\frac{d^2}{dr^2} - U(r) - \frac{\ell(\ell+1)}{r^2} + k^2 \right) u_\ell(r) = 0}$$

1. Non-interacting case: $V \equiv 0$

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

linear independent solutions:

- $F_\ell(kr) = kr\, j_\ell(kr), \qquad j_\ell(x) =$ spherical Bessel functions
- $G_\ell(kr) = kr\, n_\ell(kr), \qquad n_\ell(x) =$ spherical Neumann functions

e.g., $\quad j_0(x) = \frac{\sin x}{x}, \qquad n_0(x) = -\frac{\cos x}{x},$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}, \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

- Asymptotic behavior:
  - Bessel: $j_\ell(x \to 0) \propto x^\ell, \qquad j_\ell(x \to \infty) \to \frac{\sin(x - \ell\frac{\pi}{2})}{x}$
  - Neumann: $n_\ell(x \to 0) \propto \frac{1}{x^{\ell+1}}, \qquad n_\ell(x \to \infty) \to -\frac{\cos(x - \ell\frac{\pi}{2})}{x}$

  diverge at the origin → not suitable (see below)

- Normalizability:

$$\int d^3r\, |\psi_{\ell m}|^2 \propto \int_0^\infty r^2\, dr\, |R_\ell|^2 = \int_0^\infty dr\, |u_\ell|^2 \propto \begin{cases} \int dr\, r^2\, j_\ell^2(kr) \\ \int dr\, r^2\, n_\ell^2(kr) \end{cases}$$

$\Rightarrow$ The n_ℓ are not normalizable for $\ell \geq 1$.

- Special case $\ell = 0$:
  - $G_0(kr) = kr\, n_0(kr) = -\cos(kr) \quad \Rightarrow \quad \left(\frac{d^2}{dr^2} + k^2\right) G_0(kr) = 0$

    i.e., $G_0(kr)$ solves the equation for the radial wave function $u_0(r)$. ✓
  - total wave function: $\psi_{00}(\vec{r}) = \frac{u_0}{r} Y_0^0(\theta, \varphi) = \frac{1}{\sqrt{4\pi}} \frac{G_0}{r} = -\frac{1}{\sqrt{4\pi}} \frac{\cos(kr)}{r}$
  - behavior at the origin: $\psi_{00}(\vec{r} \to \vec{0}) \to -\frac{1}{\sqrt{4\pi}} \frac{1}{r}$
  - reminder: $\Delta \frac{1}{r} = -4\pi\, \delta^3(\vec{r})$ (cf. Poisson equation in electrostatics)

  $\Rightarrow$ $\psi_{00}(\vec{r})$ solves the free Schrödinger equation everywhere except the origin!

→ Allowed solutions of the radial equation for $V \equiv 0$:

$$u_\ell^{(0)}(r) = \mathcal{N} F_\ell(kr) = \mathcal{N}\, kr\, j_\ell(kr) \stackrel{r\to\infty}{\longrightarrow} \mathcal{N} \sin(kr - \ell\frac{\pi}{2})$$

2. Spatially localized potential:

$$V(r) \begin{cases} = 0 & \text{(or negligible) for } r > R \\ \neq 0 & \text{for small } r \end{cases}$$

- Solutions outside the potential range: $u_\ell(r > R) = A_\ell F_\ell(kr) - B_\ell G_\ell(kr)$
  - origin not contained $\Rightarrow$ Neumann functions allowed
  - solution for $r < R$ different (in particular at $r = 0$)
  - coefficients A_ℓ and B_ℓ are determined by boundary conditions at $r = R$ (continuity of u_ℓ and u'_ℓ)

- change notation: $u_\ell(r > R) = C_\ell\big(\cos\delta_\ell\, F_\ell(kr) - \sin\delta_\ell G_\ell(kr)\big)$

$$\Rightarrow \quad \left.\begin{aligned} A_\ell &= C_\ell \cos\delta_\ell \\ B_\ell &= C_\ell \sin\delta_\ell \end{aligned}\right\} \quad \Rightarrow \quad C_\ell^2 = A_\ell^2 + B_\ell^2\,, \quad \tan\delta_\ell = \tfrac{B_\ell}{A_\ell}$$

  - C_ℓ: related to the normalization
  - δ_ℓ: contains information about the potential

    $(V \equiv 0 \;\Rightarrow\; B_\ell = 0 \;\Rightarrow\; \delta_\ell = 0)$

- asymptotic behavior:

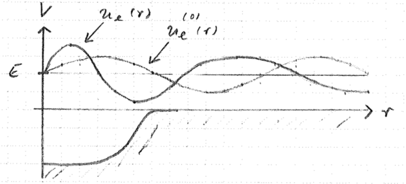
$$u_\ell(r \to \infty) = C_\ell\big(\cos\delta_\ell\, \sin(kr - \ell\tfrac{\pi}{2}) + \sin\delta_\ell \cos(kr - \ell\tfrac{\pi}{2})\big)$$
$$= C_\ell\, \sin(kr - \ell\tfrac{\pi}{2} + \delta_\ell)$$

→ δ_ℓ: "phase shift"

- **Attractive potential ($V < 0$):**

  In the potential region the wave oscillates faster than the free solution of the same energy.

  $\Rightarrow \;\; \delta_\ell > 0$



- **Repulsive potential ($V > 0$):**

  The wave oscillates slower (for $E > V$) than without potential or not at all ($E < V$)

  $\Rightarrow \;\; \delta_\ell < 0$

- **Note:** $\delta_\ell = \delta_\ell(E)$

Relation to the scattering amplitude

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- Solution of the scattering problem:

  $$\psi_{\vec{k}}(\vec{r}) = e^{ikz} + \psi_{\text{sc}}(\vec{r}) \stackrel{r\to\infty}{\longrightarrow} e^{ikz} + f_k(\theta)\,\frac{e^{ikr}}{r}$$

  Expand in a basis of angular-momentum eigenstates:

  $$\psi_{\vec{k}}(\vec{r}) = \sum_{\ell,m} c_{\ell m}\,\frac{u_\ell(r)}{r}\,Y_\ell^m(\theta,\varphi)$$

- spherically symmetric potential $V(r)$ $\Rightarrow$ $\psi_{\vec{k}}$ does not depend on φ.

  → only $Y_\ell^0 \propto P_\ell(\cos\theta)$

  → $\psi_{\vec{k}}(\vec{r}) = \sum_\ell c_\ell\,\frac{u_\ell(r)}{r}\,P_\ell(\cos\theta) \equiv \sum_\ell \psi_\ell,\quad \psi_\ell$: "partial waves"

- incoming plane wave: $e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell \, (2\ell + 1) \, j_\ell(kr) \, P_\ell(\cos\theta)$

$$\Rightarrow \quad e^{ikz} \overset{r\to\infty}{\longrightarrow} \sum_{\ell=0}^{\infty} i^\ell \, (2\ell+1) \, \frac{\sin(kr - \ell\frac{\pi}{2})}{kr} \, P_\ell(\cos\theta)$$

$$= \sum_{\ell=0}^{\infty} i^\ell \, \frac{2\ell+1}{2ik} \left(\frac{e^{i(kr-\ell\frac{\pi}{2})}}{r} - \frac{e^{-i(kr-\ell\frac{\pi}{2})}}{r} \right) P_\ell(\cos\theta)$$

(outgoing − incoming) spherical wave

- expansion of the scattering amplitude: $f_k(\theta) = \sum_{\ell=0}^{\infty} f_\ell \, P_\ell(\cos\theta), \qquad f_\ell = f_\ell(E)$

$$\Rightarrow \quad \psi_{\vec{k}}(\vec{r}) \overset{r\to\infty}{\longrightarrow} \sum_{\ell=0}^{\infty} \frac{1}{r} \left\{ i^\ell \, \frac{2\ell+1}{2ik} \left[e^{i(kr-\ell\frac{\pi}{2})} - e^{-i(kr-\ell\frac{\pi}{2})} \right] + f_\ell \, e^{ikr} \right\} P_\ell(\cos\theta)$$

$$f_\ell \, e^{ikr} = f_\ell \, e^{i\ell\frac{\pi}{2}} \, e^{i(kr-\ell\frac{\pi}{2})} = f_\ell \, i^\ell \, e^{i(kr-\ell\frac{\pi}{2})}$$

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

$$\psi_{\vec{k}}(\vec{r}) = \sum_\ell c_\ell \frac{u_\ell(r)}{r} P_\ell(\cos\theta)$$

$$\stackrel{r\to\infty}{\longrightarrow} \sum_\ell^\infty \frac{1}{r}\left\{ i^\ell \frac{2\ell+1}{2ik}\left[\left(1+\frac{2ik}{2\ell+1}f_\ell\right)e^{i(kr-\ell\frac{\pi}{2})} - e^{-i(kr-\ell\frac{\pi}{2})}\right]\right\} P_\ell(\cos\theta)$$

$$\Rightarrow \quad u_\ell(r\to\infty) \propto i^\ell \frac{2\ell+1}{2ik}\left[\left(1+\frac{2ik}{2\ell+1}f_\ell\right)e^{i(kr-\ell\frac{\pi}{2})} - e^{-i(kr-\ell\frac{\pi}{2})}\right]$$

$$\stackrel{!}{\propto} \sin(kr - \ell\tfrac{\pi}{2} + \delta_\ell)$$

$$= \frac{1}{2i}\left[e^{i\delta_\ell} e^{i(kr-\ell\frac{\pi}{2})} - e^{-i\delta_\ell} e^{-i(kr-\ell\frac{\pi}{2})}\right]$$

$$= \frac{1}{2i} e^{-i\delta_\ell}\left[e^{2i\delta_\ell} e^{i(kr-\ell\frac{\pi}{2})} - e^{-i(kr-\ell\frac{\pi}{2})}\right]$$

$$\Rightarrow \quad e^{2i\delta_\ell} = 1 + \frac{2ik}{2\ell+1} f_\ell$$

$$\Rightarrow \quad f_\ell = \frac{2\ell+1}{2ik}\left(e^{2i\delta_\ell} - 1\right) = \frac{2\ell+1}{2ik}\left(e^{i\delta_\ell} - e^{-i\delta_\ell}\right) e^{i\delta_\ell} = \frac{2\ell+1}{k}\sin\delta_\ell e^{i\delta_\ell}$$

$$\boxed{f_\ell = \frac{2\ell+1}{k} \sin\delta_\ell e^{i\delta_\ell}}$$

$$\Rightarrow \quad f_k(\theta) = \tfrac{1}{k}\sum_\ell (2\ell+1)\ \sin\delta_\ell\ e^{i\delta_\ell}\ P_\ell(\cos\theta)$$

- differential cross section:

$$\tfrac{d\sigma}{d\Omega} = \left|f_k(\theta)\right|^2 = \tfrac{1}{k^2}\sum_{\ell,\ell'} (2\ell+1)(2\ell'+1)\ \sin\delta_\ell \sin\delta'_\ell\ e^{i(\delta_\ell-\delta_{\ell'})}\ P_\ell(\cos\theta) P_{\ell'}(\cos\theta)$$

The different partial waves interfere:

The particles measured by the detector have a well-defined momentum $\hbar\vec{k}\,'$

$\Rightarrow$ no well-defined angular momentum