Quantum scattering with a spherically symmetric potential

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Scattering phenomena: background[1]

- In an idealized scattering experiment, a sharp beam of particles (A) of definite momentum **k** are scattered from a localized target (B).
- As a result of collision, several outcomes are possible:

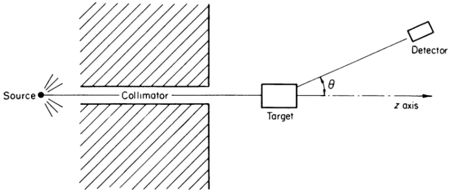


Figure: A schematic representation of a standard scattering experiment

$$A + B \longrightarrow \begin{cases} A + B & \text{elastic} \\ \left.\begin{array}{r} A + B^* \\ A + B + C \end{array}\right\} & \text{inelastic} \\ C & \text{absorption} \end{cases}$$

[1] R. M. Thaler L. S. Rodberg. *Introduction to the Quantum Theory of Scattering*. Academic Pr, 1967.

Scattering phenomena: differential and total cross section

- Detector measures the number of particles per unit time, $Nd\Omega$, scattered into an element of solid angle $d\Omega$ in direction (θ, ϕ).
- The number is proportional to the incident flux of particles, j_{inc}, defined as the number of particles per unit time crossing a unit area normal to direction of incidence.
- Collisions are characterised by the **differential cross section** defined as the ratio of the number of particles scattered into direction (θ, ϕ) per unit time per unit solid angle, divided by the incident flux

$$\frac{d\sigma}{d\Omega} = \frac{N}{j_{\text{inc}}}$$

- From the differential, we can obtain the **total cross section** by integrating over all solid angles

$$\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta$$

Lectures recap

The Hamiltonian for a system of two interacting particles

$$\hat{H} = \frac{\mathbf{P}_A^2}{2m_A} + \frac{\mathbf{P}_B^2}{2m_B} + V_{AB}$$

Separating out the motion of the center of mass

$$\mathbf{r} \equiv \mathbf{r}_A - \mathbf{r}_B, \quad \mathbf{R} \equiv \frac{m_A \mathbf{r}_A + m_B \mathbf{r}_B}{m_A + m_B}$$

$$\left[-\frac{\hbar^2}{2M}\nabla_R^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(r) \right] \Psi(\mathbf{r}_A, \mathbf{r}_B) = E\Psi(\mathbf{r}_A, \mathbf{r}_B),$$

where

$$M = m_A + m_B, \quad \mu = \frac{m_A m_B}{m_A + m_B}$$

It permits a separation of the variables **R** and **r**

$$\Psi(\mathbf{r}_A, \mathbf{r}_B) = \Phi(\mathbf{R})\psi(\mathbf{r})$$
$$-\frac{\hbar^2}{2M}\nabla_R^2\Phi(\mathbf{R}) = E_{\text{cm}}\Phi(\mathbf{R})$$
$$\left\{-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right\}\psi(\mathbf{r}) = E_{\text{rel}}\psi(\mathbf{r}) \tag{1}$$

where

$$E = E_{\text{cm}} + E_{\text{rel}} \tag{2}$$

Stationary scattering theory

Asymptotically ψ must consist of an incoming wave and an outgoing spherical wave centered about the origin of the scattering field. The amplitude of the scattered wave depends on two angles θ and ϕ.

$$\psi(\mathbf{r}) \xrightarrow[r \to \infty]{} \exp\left(i\left(\mathbf{k} \cdot \mathbf{r}\right)\right) + \frac{\exp\left(ikr\right)}{r} f(\theta, \phi) = \psi_0 + \psi_s$$

Asymptotic behavior of the cross sections can be obtained by considering the particle flux. The particle flux density is

$$\mathbf{j} = -\frac{i\hbar}{2\mu}\left(\psi^* \nabla \psi - \psi \nabla \psi^*\right)$$

Incident plane wave ψ_0 and scattered wave ψ_s yield corresponding flux densities

$$\mathbf{j}_0 = \frac{\hbar \mathbf{k}}{\mu}, \quad \mathbf{j}_s = \frac{\hbar \mathbf{k}}{\mu r^2} |f(\theta, \phi)|^2.$$

Following the definition of the differential scattering cross section

$$\frac{d\sigma}{d\Omega} = \frac{\text{particle flux scattered into unit solid angle } d\Omega}{\text{incident particle flux density}} = |f(\theta, \phi)|^2$$

For a spherically symmetric potential, the solution of the Schroedinger equation can always be written as

$$\psi(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm} \frac{u_l(r)}{r} Y_l^m(\theta, \phi)$$

where u_l satisfies the radial Schroedinger equation

$$\left\{ \frac{\hbar^2}{2\mu} \frac{d^2}{dr^2} + \left[E - V(r) - \frac{\hbar^2 l(l+1)}{2\mu r^2} \right] \right\} u_l(r) = 0. \quad (3)$$

Outside the well, the solution u_l can be written as a linear combination of *spherical Bessel* and *spherical Neumann* functions of order l:

$$u_l(r) = Arj_l(kr) + Brn_l(kr), \quad k = \sqrt{2\mu E}\hbar,$$

$$\text{where} \quad j_l(x) = (-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\sin x}{x},$$

$$\text{and} \quad n_l(x) = -(-x)^l \left(\frac{1}{x} \frac{d}{dx} \right)^l \frac{\cos x}{x}.$$

u_l approaches a sine-wave form for large r and the phase of this wave is determined by δ_l[2]

$$u_l(r) \sim \sin(kr - l\pi/2 + \delta_l).$$

Phase-shifts δ_l determine scattering amplitude $f(\theta)$ by relation

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)(S_l - 1)P_l(\cos\theta), \quad S_l = \exp\left(2i\delta_l\right).$$

Substituting previous relation into definition of the total cross section we get

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l.$$

[2] Лифшиц Е.М. Ландау Л.Д. *Теоретическая физика. В 10 томах. Том 03. Квантовая механика: нерелятивистская теория*. ФМЛ, 2002.

Numerical procedure for calculating cross sections[3]

Select some definite value of energy E and for all values of angular momentum l from 0 to $l_{\max}$:

1. Integrate the radial Schroedinger equation to some $r_{\max}$ value
2. Match the numerical solution with spherical Bessel and Neumann functions to determine phase shift δ_l
3. Calculate contribution to cross section

[3] J. M. Thijssen. *Computational Physics*. Cambridge University Press, 1999.

Numerov's method for the radial Schroedinger equation

Define auxiliary function

$$F(l,r,E) = V(r) + \frac{\hbar^2 l(l+1)}{2\mu r^2} - E$$

so that the radial Schroedinger equation now reads

$$\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u(r) = F(l,r,E)u(r).$$

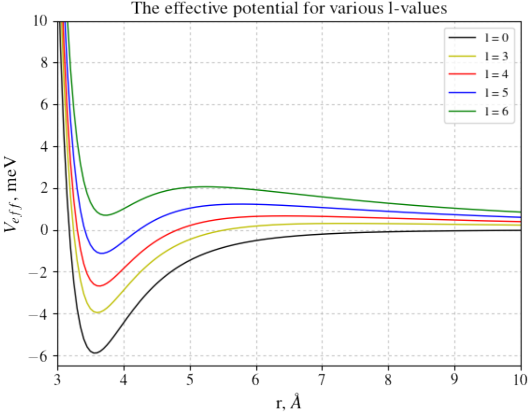
Numerov's algorithm makes use of the special structure of this equation to solve it with an error of order h^6. For $\hbar^2/2\mu \equiv 1$ it reads:

$$\omega(r+h) = 2\omega(r) - \omega(r-h) + h^2 F(l,r,E)u(r)$$
$$u(r) = \left(1 - \frac{h^2}{12}F(l,r,E)\right)^{-1}\omega(r).$$

Interaction potential

Model system: H-Kr. The two-atom interaction potential is often modelled by the Lennard-Jones potential of the following form:

$$V_{\mathrm{LJ}}(r) = \varepsilon \left[\left(\frac{\rho}{r} \right)^{12} - 2 \left(\frac{\rho}{r} \right)^{6} \right], \quad \varepsilon = 5.9\text{meV}, \quad \rho = 3.57\text{Å}.$$

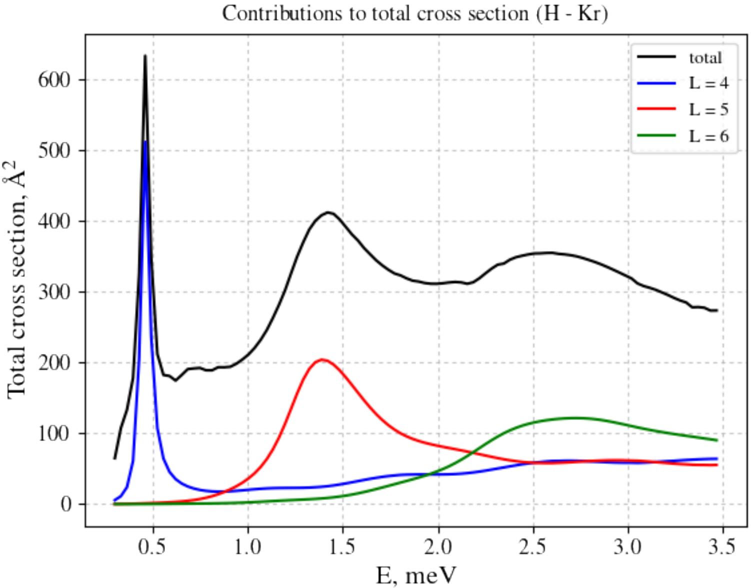


The first two points can be calculated in the following way, assuming the asymptotic form for $r \to 0$:

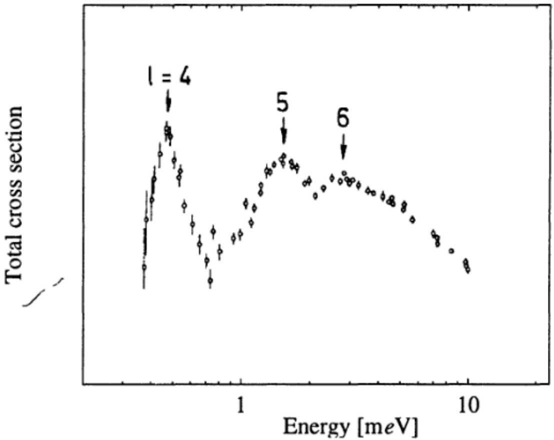
$$\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u(r) \approx \varepsilon\left(\frac{\rho}{r}\right)^{12}u(r),$$
$$u(r) \approx \exp\left(-\sqrt{\frac{2\mu\varepsilon\rho^{12}}{25\hbar^2}}r^{-5}\right).$$

Matching the numerical solution to asymptotic solution is done via two point method

$$\tan\delta_l = \frac{Kj_l^{(1)} - j_l^{(2)}}{Kn_l^{(1)} - n_l^{(2)}} \quad \text{with} \quad K = \frac{r_1 u_l^{(2)}}{r_2 u_l^{(1)}}.$$


Contributions to total cross section (H - Kr)
total
L = 4
L = 5
L = 6
Total cross section, Å^2
0
100
200
300
400
500
600
0.5
1.0
1.5
2.0
2.5
3.0
3.5
E, meV

Experimental results[4]



[4] J Peter Toennies, Wolfgang Welz, and Günther Wolf. "Molecular beam scattering studies of orbiting resonances and the determination of van der Waals potentials for H–Ne, Ar, Kr, and Xe and for H2–Ar, Kr, and Xe". In: *The Journal of Chemical Physics* 71.2 (1979), pp. 614–642.

Radial wavefunctions in the vicinity of the resonance L = 4