Exercitation

Scattering processes

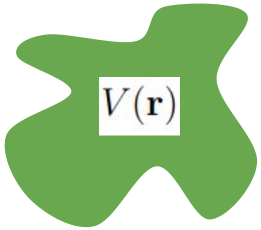
Partial Wave Analysis

Analytical and numerical determination of phase shifts and cross sections

Motivation

Scattering processes are the primary way we learn about distributions, shapes, and potential energies for nuclear systems.

We will solve the Schrodinger equation in the continuum for *elastic* scattering from a potential of a *finite* extent.



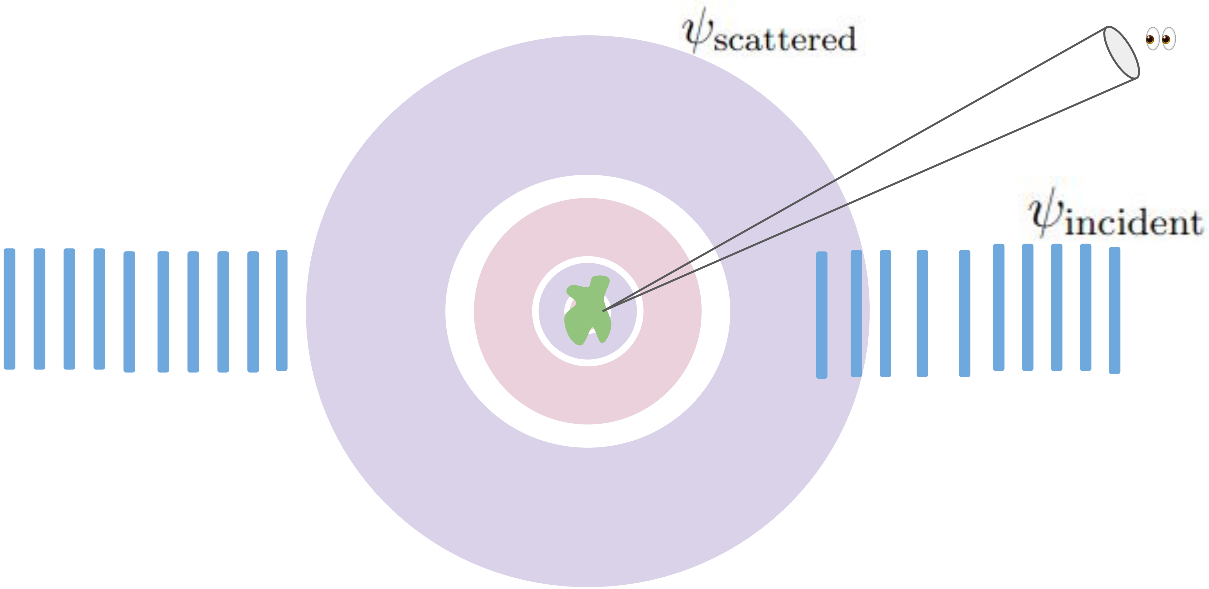
$$\lim_{r \to \infty} r\, V(\mathbf{r}) = 0$$

$$E = \frac{\hbar^2 k^2}{2\, m}$$

$$\left[-\frac{\hbar^2}{2\, m} \nabla^2 + V(\mathbf{r}) \right] \psi = E \psi$$

$$\psi = \psi_{\text{incident}} + \psi_{\text{scattered}}$$

$$\psi \xrightarrow[r\to\infty]{} \boxed{e^{i\mathbf{k}\cdot\mathbf{r}}} + \boxed{\frac{e^{i\,kr}}{r}} f_k(\theta,\phi)$$



Scattering Amplitude and Cross Section

$$\psi \xrightarrow[r\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{i\,kr}}{r} f_k(\theta,\phi)$$

The scattering amplitude depends on V(**r**) and encodes the effects induced by the potential on the scattered wave.

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

Scattering by a Central Potential

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

We can express the solution of the Schrodinger equation in terms of eigenstate of the angular momentum and study the effect of the potential in each partial wave.

$$\psi(r,\theta,\phi) = R(r)\,Y_\ell^m(\theta,\phi)$$

R(r) satisfies the radial equation.

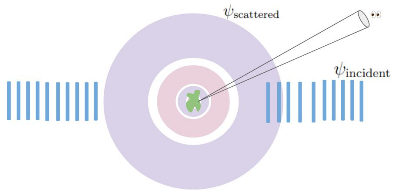
Partial wave expansion

$$\psi \xrightarrow[r\to\infty]{} e^{i\mathbf{k}\cdot\mathbf{r}} + \frac{e^{i\,kr}}{r} f_k(\theta)$$

$$e^{i\,\mathbf{k}\cdot\mathbf{r}} = \sum_{\ell=0}^{\infty} i^{\ell}\,(2\,\ell+1)\,j_\ell(k\,r)P_\ell(\cos\theta)$$

$$f_k(\theta) = \sum_{\ell=0}^{\infty}(2\,\ell+1)\;f_\ell(k)\;P_\ell(\cos\theta)$$

Note that the scattering amplitude depends only on theta.



Partial Wave Amplitude and Cross Section

$$f_k(\theta) = \sum_{\ell=0}^{\infty} (2\,\ell + 1)\, f_\ell(k)\, P_\ell(\cos\theta)$$

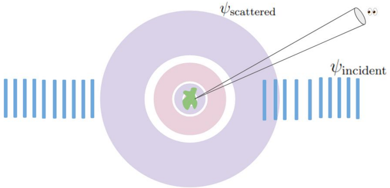
$f_\ell(k)$ is the partial wave amplitude, encoding the effect of the interaction in each partial wave.

$$\sigma = 4\,\pi \sum_{\ell=0}^{\infty} (2\,\ell + 1) |f_\ell(k)|^2$$

Asymptotic limit

$$e^{i\,\mathbf{k}\cdot\mathbf{r}} \xrightarrow[r\to\infty]{} \sum_{\ell=0}^{\infty} \frac{(2\,\ell+1)\,P_\ell(\cos\theta)}{2\,i\,k} \left[\frac{e^{i\,kr}}{r} - (-1)^\ell\,\frac{e^{-i\,kr}}{r}\right]$$

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

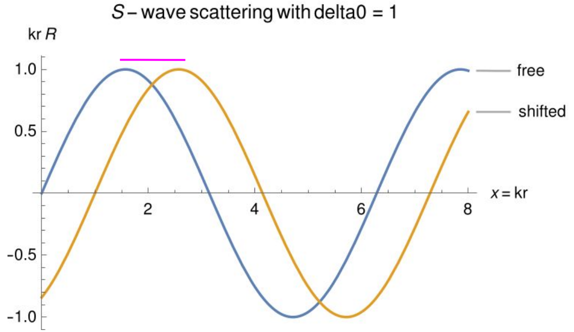


Phase Shifts and Cross Section

$$f_\ell(k) = \frac{e^{i\delta_\ell}\,\sin\delta_\ell}{k}$$

$$\psi \xrightarrow[r\to\infty]{} \sum_{\ell=0}^{\infty} \frac{(2\,\ell+1)\,P_\ell(\cos\theta)}{2\,i\,k}\left[e^{2\,i\,\delta_\ell}\,\frac{e^{i\,kr}}{r} - (-1)^\ell\,\frac{e^{-i\,kr}}{r}\right]$$

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

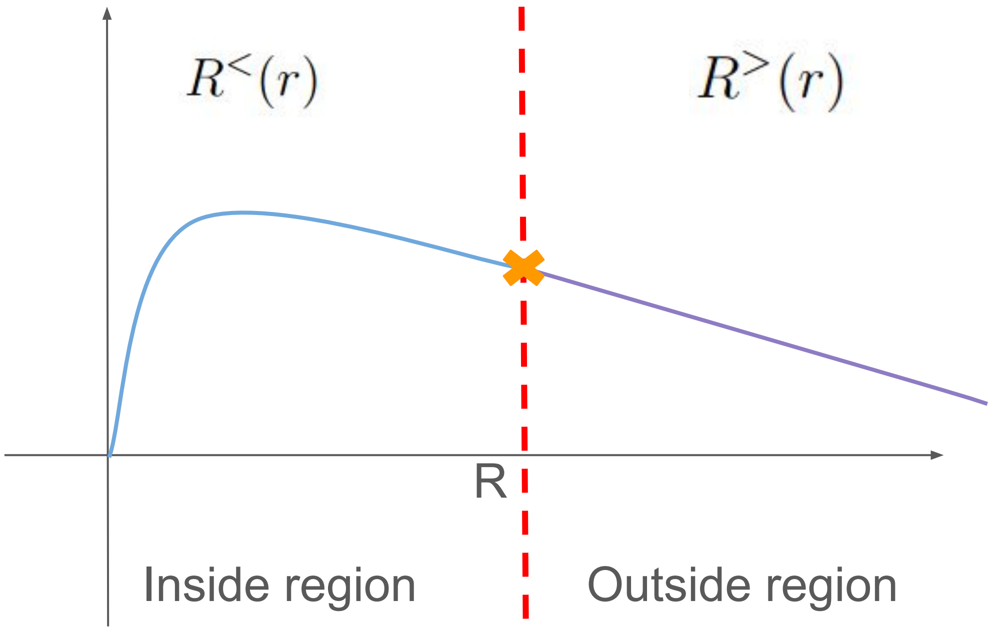


Analytical solution

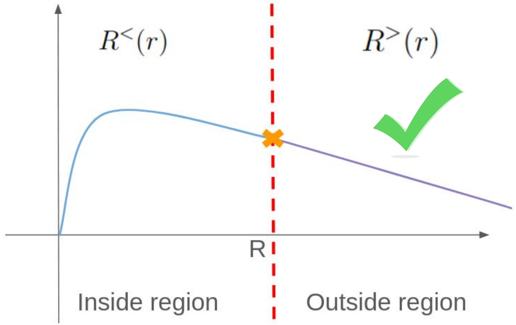
R ~ where the potential fades away

$$R^{<}(r) = R^{>}(r)\Big|_{r=R}$$

$$R^{<\prime}(r) = R^{>\prime}(r)\Big|_{r=R}$$



Outside Region



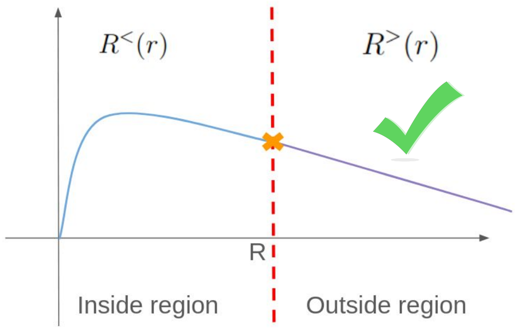
$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$$

The solution of the Schrodinger equation that matches the asymptotic behaviour of ψ as $r\to\infty$ is

$$R^{>}(r) = e^{i\delta_\ell}\left[\cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, n_\ell(kr)\right]$$

$$\psi(r,\theta,\phi) = R(r)\,Y_\ell^m(\theta,\phi)$$

Inside Region

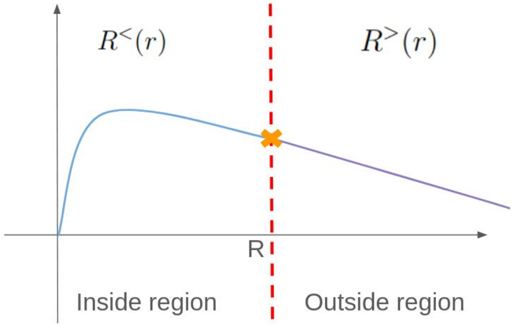


$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right]\psi = E\psi$$

$$\psi(r,\theta,\phi) = R(r)\,Y_\ell^m(\theta,\phi)$$

Solve for R(r)

Phase shifts



✖

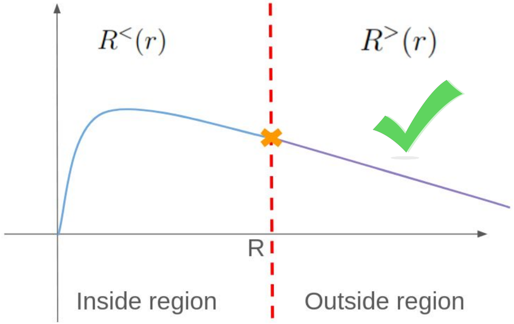
$$R^<(r) = R^>(r)\Big|_{r=R}$$

$$R^{<\prime}(r) = R^{>\prime}(r)\Big|_{r=R}$$

$$\tan\delta_\ell = \frac{kR\, j_\ell'(kR) - \beta_\ell\, j_\ell(kR)}{kR\, n_\ell'(kR) - \beta_\ell\, n_\ell(kR)}$$

$$\beta_\ell = r\frac{R'(r)}{R(r)}\Big|_{r=R}$$

Inside Region

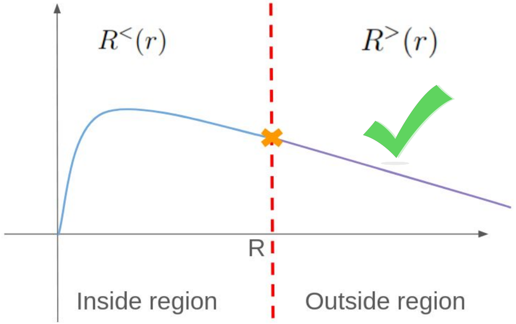


$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right]\psi = E\psi$$

$$u(r) = r\,R(r)$$

$$u(0) = 0$$

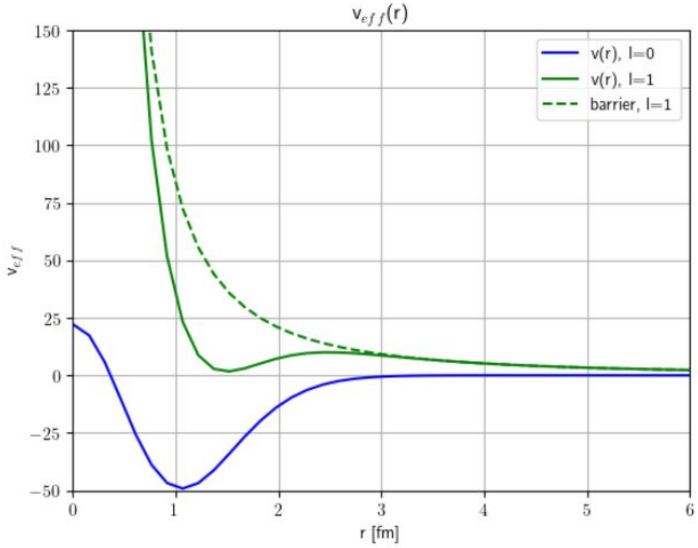
$$v(r) = \frac{2m}{\hbar^2}V(r)$$



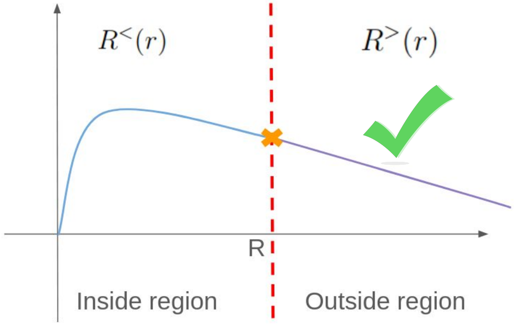
Inside Region - Radial Equation

$$u'' + \left[k^2 - v(r) - \frac{\ell(\ell+1)}{r^2}\right] u = 0$$

$$v_{\text{eff}}(r) = v(r) + \frac{\ell(\ell+1)}{r^2}$$



Inside Region - Radial Equation



$$u_\ell'' + \left[k^2 - v(r) - \frac{\ell(\ell+1)}{r^2}\right] u_\ell = 0$$

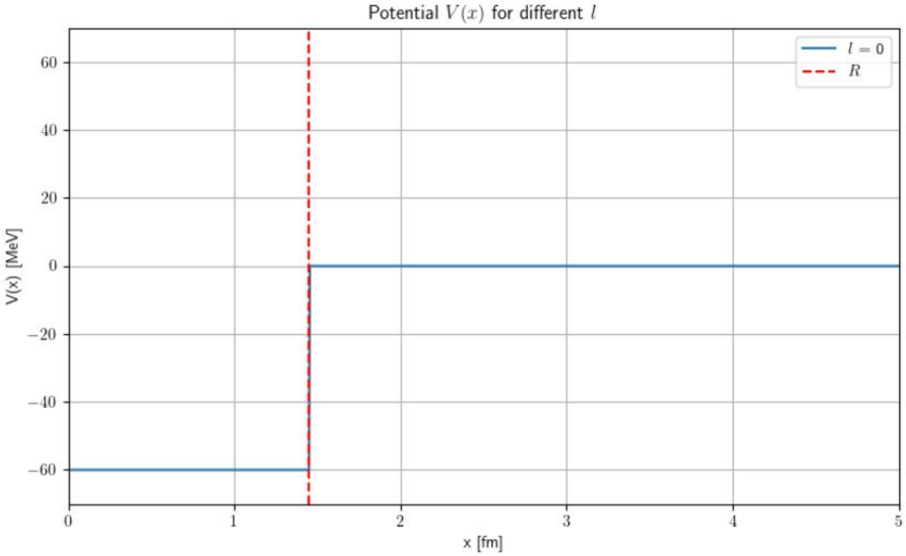
In the limit of r going to 0, and assuming that the barrier dominates over v(r) in this limit, then

$$u_\ell'' + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right] u_\ell = 0$$

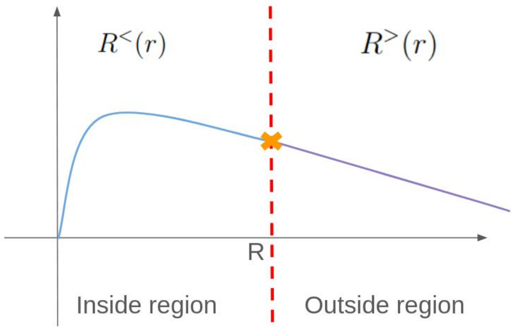
$$u_\ell(r) \xrightarrow[r\to 0]{} r^{\ell+1}$$

Analytical Example: Square Well

$$V(r) = \begin{cases} -V_0 & \text{for } r \leq R \\ 0 & \text{otherwise} \end{cases}$$



Outside region

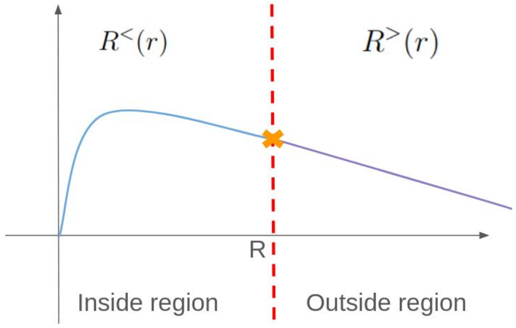


$$R^>(r) = e^{i\delta_\ell}\left[\cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, n_\ell(kr)\right]$$

$$u(r) = r\,R(r)$$

$$\boxed{u_0 = \sin(kr + \delta_0)}$$

Inside region



In the inside region in the S-wave channel (l=0) the radial equation is

$$u_0'' + \left[k^2 - v(r)\right] u_0 = 0$$

or in a more compact notation

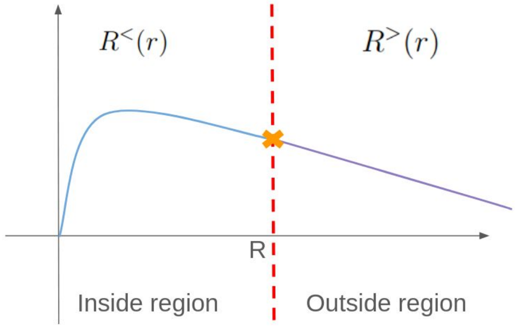
$$u_0'' + k' u_0 = 0$$

$$k' = k^2 + \frac{2m}{\hbar^2} V_0$$

with solution

$$u_0 = A \sin k' r$$

Matching



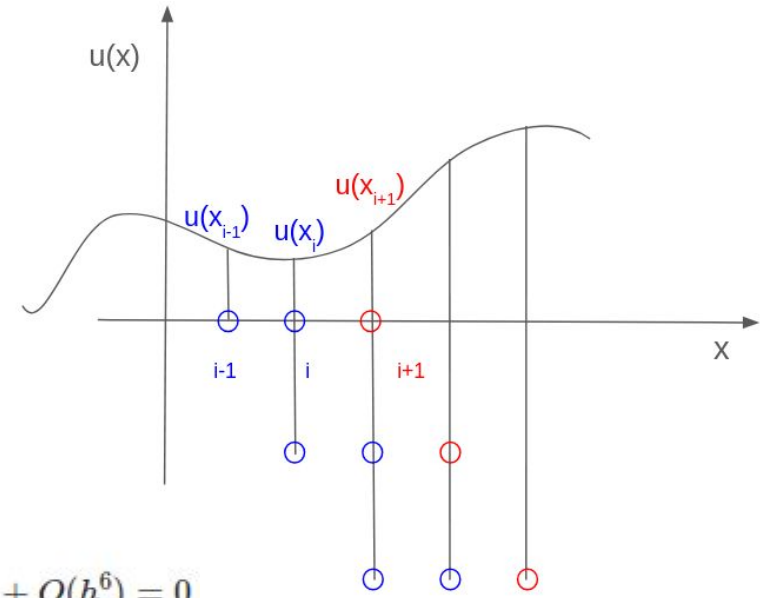
$$u^<(r) = u^>(r)\big|_{r=R}$$

$$u^{<\prime}(r) = u^{>\prime}(r)\big|_{r=R}$$

$$\tan\delta_0 = \frac{\cos kR \sin k'R - \frac{k'}{k}\cos k'R \sin kR}{\frac{k'}{k}\cos kR \cos k'R + \sin k'R \sin kR}$$

We will use this result to validate our numerical code that calculates phase shifts and cross sections.

Numerov Algorithm



$$u''(r) + K(r)u(r) = 0$$

$$u_{i+1}\left(1+\frac{h^2}{12}K_{i+1}\right) - u_i\left(2-\frac{5\,h^2}{6}K_i\right) + u_{i-1}\left(1+\frac{h^2}{12}K_{i-1}\right) + O(h^6) = 0$$

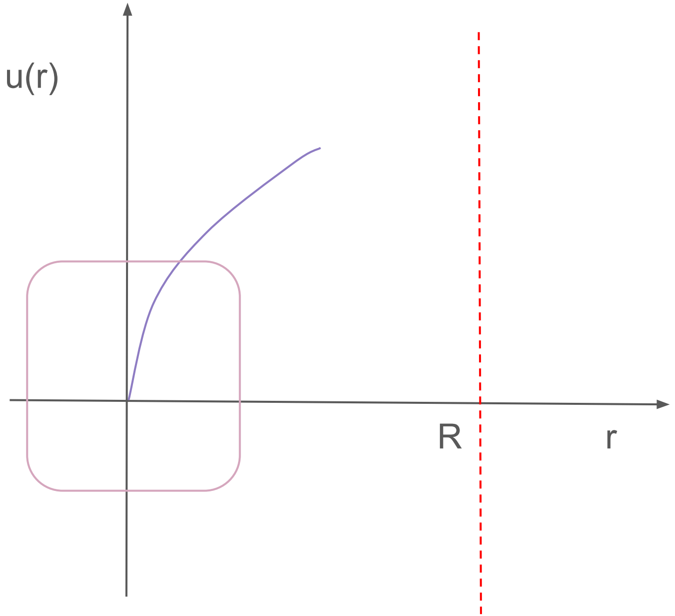
$$u_{i+1} = \frac{u_i\left(2-\frac{5\,h^2}{6}K_i\right) - u_{i-1}\left(1+\frac{h^2}{12}K_{i-1}\right)}{\left(1+\frac{h^2}{12}K_{i+1}\right)}$$

Numerical Solution: Wave Function

$$u''(r) + K(r)u(r) = 0$$

$$K(r) = \frac{2\mu}{\hbar^2}[E - V(r)] - \frac{\ell(\ell+1)}{r^2} = k'^2 - \frac{\ell(\ell+1)}{r^2}$$

$$u_\ell(r) \xrightarrow[r \to 0]{} r^{\ell+1}$$



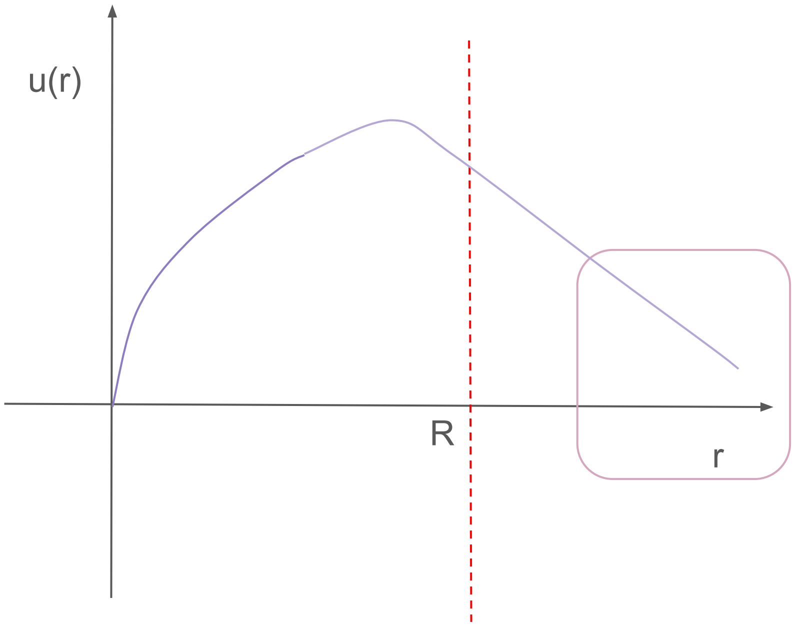
Use Numerov to construct the wave function in each l-channel and for each energy.

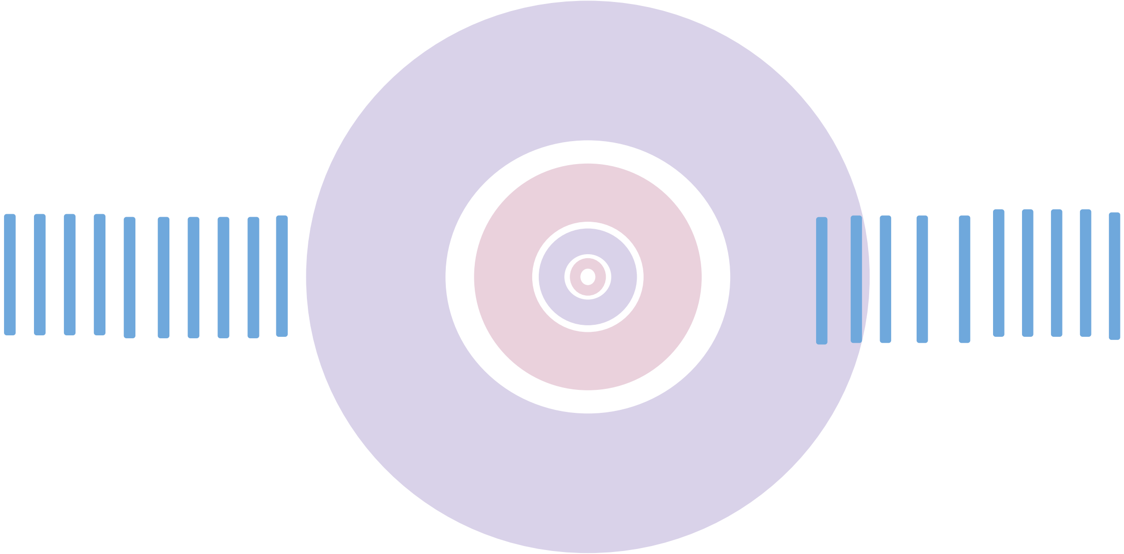
Numerical Solution: Phase shifts

$$u(r) \to r\left[\cos\delta_\ell\, j_\ell(kr) - \sin\delta_\ell\, n_\ell(kr)\right]$$

$$\tan\delta_\ell = \frac{j_\ell(kr_1) - \alpha\, j_\ell(kr_2)}{n_\ell(kr_1) - \alpha\, n_\ell(kr_2)}$$

$$\alpha = \frac{u(r_1)\, r_2}{u(r_2)\, r_1}$$





To dos

Now we play with the notebook `PhaseShifts’.

You will then write your own code to solve the assigned exercise.