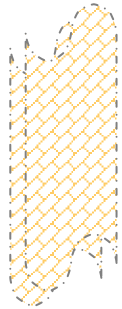
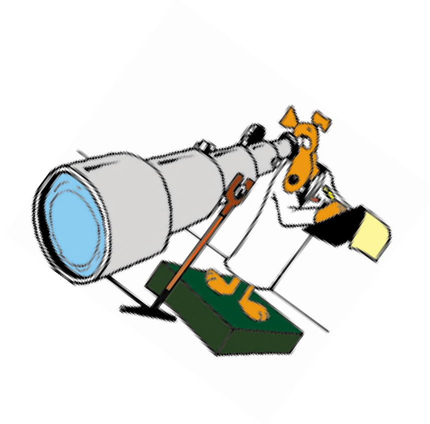
Scattering is in general time process





One make use of conservation laws to simplify the problem to solve:

- Hamiltonian is Hermitian
- Symmetry with respect to particle permutation
- Translational invariance
- Rotational invariance

$$\frac{\partial A}{\partial t} \equiv 0 \quad \textit{number of particles is conserved}$$

$$\Psi(\ldots,\alpha_i,\alpha_j,\ldots) = \pm\Psi(\ldots,\alpha_j,\alpha_i,\ldots) \quad \alpha_i = \vec{r}_i, \vec{p}_i, \vec{l}_i, \vec{\sigma}_i, \vec{\tau}_i$$

$$\frac{\partial \sum_{i=1}^{A} \vec{p}_i}{\partial t} \equiv 0; \quad \frac{\partial \sum_{i=1}^{A} \varepsilon_i}{\partial t} \equiv 0$$

$$[\hat{H},\hat{J}] \equiv 0; \quad \vec{J} = \sum_{i=1}^{A} \vec{l}_i + \vec{s}_i; \quad \vec{l} = \vec{p}_i \times \vec{r}_i$$

Approximate symmetries:

- Galilean invariance
- Mirror invariance
- Time reversal invariance
- Isospin invariance

$$\frac{\partial V}{\partial \vec{R}} \equiv 0; \quad \frac{\partial V}{\partial \vec{P}} \equiv 0; \quad \vec{R} = \frac{\sum_{i=1}^{A} m_i \vec{r}_i}{\sum_{i=1}^{A} m_i}; \quad \vec{P} = \sum_{i=1}^{A} \vec{p}_i$$

$$\Psi(\alpha_i,\alpha_j,\ldots) = \Pi\Psi(\hat{\Pi}\alpha_i,\hat{\Pi}\alpha_j,\ldots); \quad \Pi = \pm 1;$$

$$a + b \Leftrightarrow c + d$$

$$V_{nn}(\alpha_i) \approx V_{pp}(\alpha_i) \approx V_{np}(\alpha_i); \quad [\hat{H},\hat{T}] \approx 0$$

In non-relativistic QM one has to solve stationary Schrödinger eq.

$$(E-H)\Psi(\alpha_i,\alpha_j,....,\alpha_n)=0$$

2-particle case (partial wave Schrödinger eq):

$$\left(E+\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}-V_\ell(r)\right)\psi_\ell(r)=0; \qquad \vec{r}=\vec{r}_2-\vec{r}_1; \qquad E=\frac{\hbar^2}{2\mu}k^2$$

with boundary condition

Bound states:

$$\begin{cases}\psi_\ell(0)=0\\ \psi_\ell(r)\xrightarrow[r\to\infty]{}0\end{cases}$$

Scattering states:

$$\begin{cases}\psi_\ell(0)=0\\ \psi_\ell(r)\xrightarrow[r\to\infty]{}\hat{j}_\ell(r)+kf_\ell(k)\mathrm{e}^{i(kr-\ell\frac{\pi}{2})}\end{cases}$$

$$\xrightarrow[r\to\infty]{}\hat{j}_\ell(kr)+kf_\ell(k)\hat{h}_\ell^+(kr)$$

$$\xrightarrow[r\to\infty]{}\hat{h}_\ell^-(kr)-S_\ell(k)\hat{h}_\ell^+(kr)$$

$$\xrightarrow[r\to\infty]{}\hat{j}_\ell(kr)+tg\delta_\ell(k)\hat{n}_\ell(kr)$$

$$\xrightarrow[r\to\infty]{}\sin(kr-\frac{1}{2}\ell\pi+\delta_\ell(k))$$

$$f(\vec{k}',\vec{k})=\sum_{\ell=0}^{\infty}(2\ell+1)f_\ell(k)P_\ell(\hat{k}'\cdot\hat{k})$$

$$f_\ell(k)=\frac{S_\ell(k)-1}{2ik}=\frac{e^{i\delta_\ell(k)}\sin\delta_\ell(k)}{k}$$

$$S_\ell(k)=e^{2i\delta_\ell(k)}$$

Analogous formulation if Coulomb is present, however:

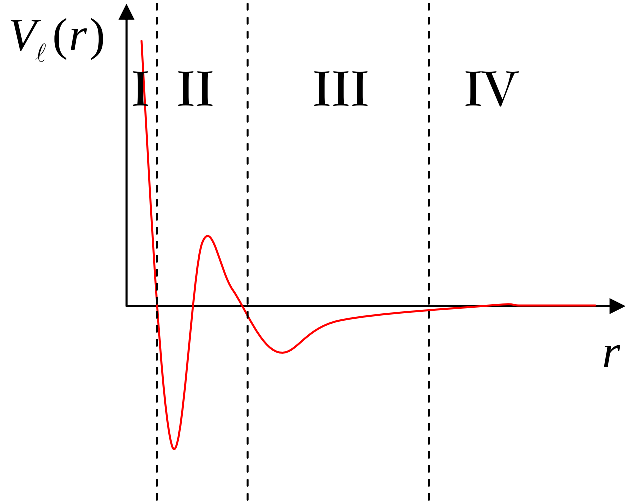
$$\hat{j}_\ell\to F_\ell^C$$

$$\hat{n}_\ell\to G_\ell^C$$

$$\hat{h}_\ell^\pm\to\hat{u}_\ell^\pm$$

How to solve differential equation(s) with boundary condition?

$$\left(E+\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}-V_\ell(r)\right)\psi_\ell(r)=0 \qquad \vec{r}=\vec{r}_2-\vec{r}_1$$



• Potential may contain several zones of different behavior/importance

• Systems wave function may be concentrated in one of the regions

Therefore it may be interesting to solve the problem on the grid by smartly distributing the points (i.e. putting more points in region of larger importance/variation)

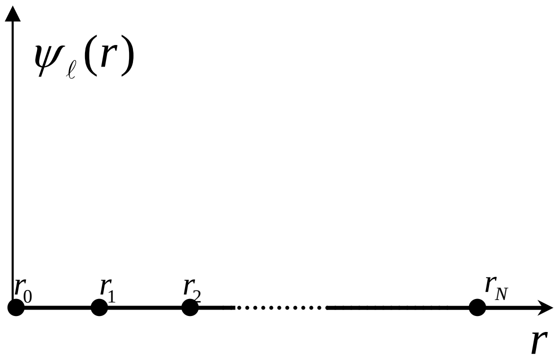
Guideline:

1) subdivide the domain into a number of subintervals (a grid)
2) expand the wave function on this grid
3) require differential eq. to be satisfied only in a set of well-chosen points
4) satisfy boundary conditions on the outside borders of the grid
5) solve resultant linear algebra problem

Numerov method

$$\left(E+\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}-V_\ell(r)\right)\psi_\ell(r)=0$$

(1)



(2)

$$\psi_\ell(r)=\begin{bmatrix}\psi_\ell(r_0)\\ \psi_\ell(r_1)\\ \psi_\ell(r_2)\\ \vdots\\ \psi_\ell(r_N)\end{bmatrix}=\begin{bmatrix}C_0\\ C_1\\ C_2\\ \vdots\\ C_N\end{bmatrix}$$

(3) Expand in Maclaurin series around point i: $\psi_\ell(r)=a_i+b_i(r-r_i)+c_i(r-r_i)^2+o((r-r_i)^3)$

$$\begin{cases}\psi_\ell(r_{i-1})=a_i-b_i(r_i-r_{i-1})+c_i(r_i-r_{i-1})^2+o((r_i-r_{i-1_i})^3)\\ \psi_\ell(r_i)=a_i\\ \psi_\ell(r_{i+1})=a_i+b_i(r_{i+1}-r_i)+c_i(r_{i+1}-r_i)^2+o((r_{i+1}-r_i)^3)\end{cases}\Rightarrow\begin{cases}a_i=C_i\\ \left.\frac{d^2}{dr^2}\psi_\ell(r)\right|_{r=r_i}=2c_i\end{cases}$$

$$\text{if}\quad r_{i+1}-r_i=r_i-r_{i-1}\qquad \left.\frac{d^2}{dr^2}\psi_\ell(r)\right|_{r=r_i}=\frac{C_{i+1}+C_{i-1}-2C_i}{(r_i-r_{i-1})^2}$$

$$\left(E+\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}-V_\ell(r)\right)\psi_\ell(r)=0\ \Rightarrow\begin{bmatrix} & & 0 & 0 & 0\\ h_{10} & h_{11} & h_{12} & 0 & 0\\ 0 & h_{21} & h_{22} & h_{23} & 0\\ 0 & 0 & \vdots & \vdots & \vdots\\ 0 & 0 & 0 & \vdots & \vdots\end{bmatrix}\begin{bmatrix}C_0\\ C_1\\ C_2\\ \vdots\\ \vdots\end{bmatrix}$$

Numerov method

(4)

Bound states:

$$\begin{cases} \psi_\ell(0)=0 \\ \psi_\ell(r)\xrightarrow[r\to\infty]{} 0 \end{cases}$$

Scattering states:

$$\begin{cases} \psi_\ell(0)=0 \\ \psi_\ell(r)\xrightarrow[r\to\infty]{} \hat{j}_\ell(r)+kf_\ell(k)\mathrm{e}^{i(kr-\ell\frac{\pi}{2})} \end{cases}$$

$$\psi_\ell(r)=\begin{bmatrix} \psi_\ell(r_0) \\ \psi_\ell(r_1) \\ \psi_\ell(r_2) \\ \vdots \\ \psi_\ell(r_N) \end{bmatrix}=\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \\ C_N \end{bmatrix}$$

Startpoint of the grid

$$\psi_\ell(0)=0 \quad \Rightarrow \quad C_0=0$$

Endpoint of the grid

a) Remplace the last equation by the boundary condition (easy for the bound state)

b) Use the trick: C_1=1 and get iteratively C_2,C_3,….

(5)

Remains to solve corresponding linear algebra problem

$$[A]C^{(i)}=E^{(i)}C^{(i)}$$

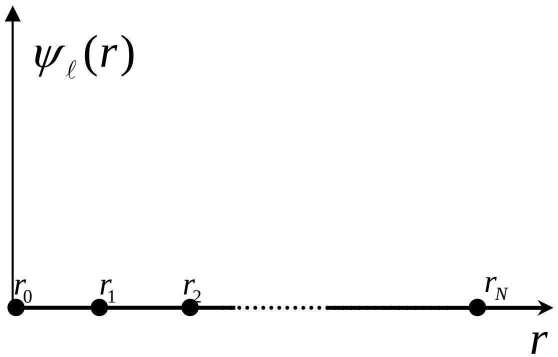
For bound states eigenvalue-eigenvector problem of size N*N

$$[A]C=X$$

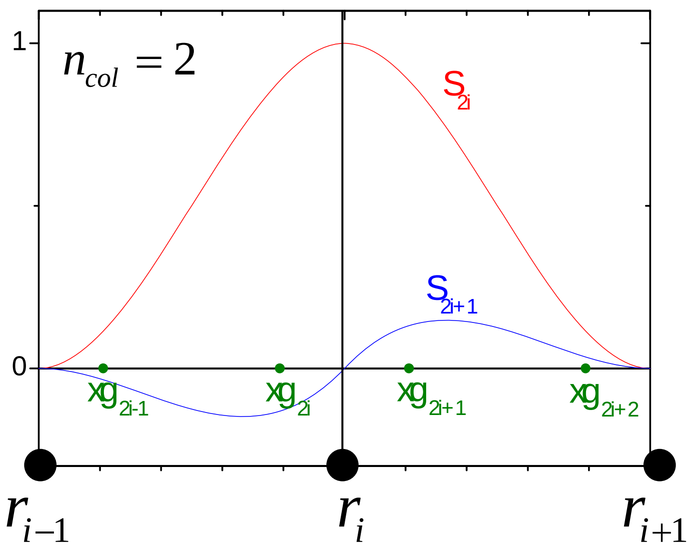
For scattering states system of N linear equations

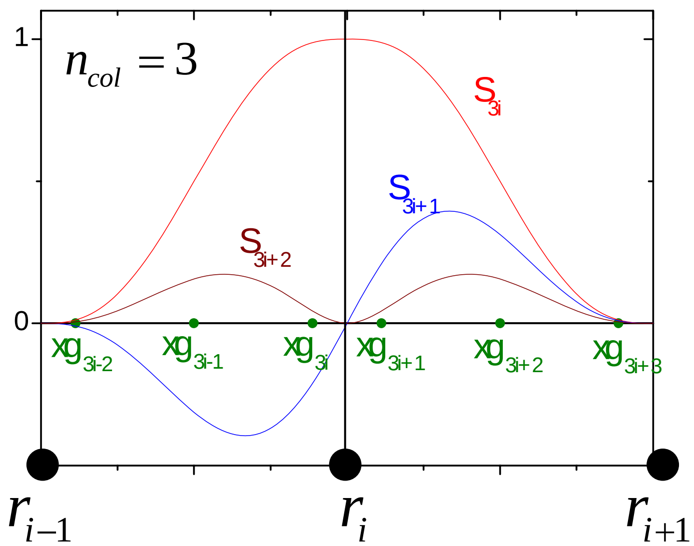
Collocation method (C. de Boor, *A Practical Guide to Splines*, Springer, Berlin 1978)

(1)



(2) We associate n_{col} local orthogonal polynomials of order $2n_{col}$ -1 with each grid point:

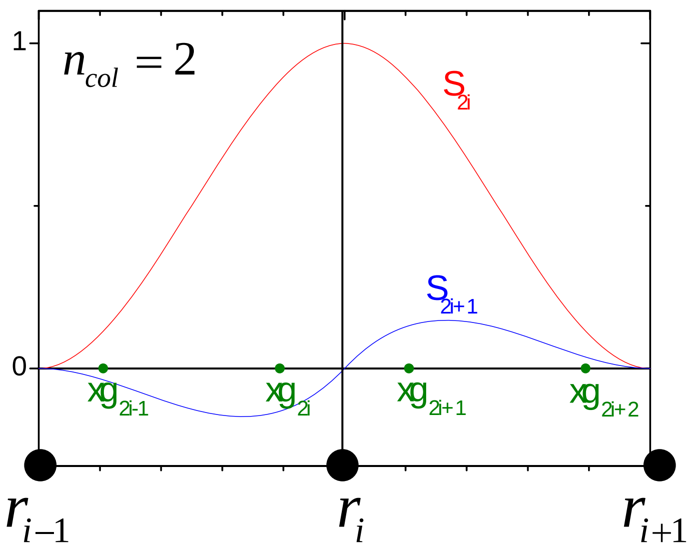




$$\psi_\ell(r) = \sum_{k=0}^{n_{col}(N+1)-1} C_k S_k(r) \quad \Longrightarrow \quad \begin{aligned} \frac{d}{dr}\psi_\ell(r) &= \sum_{k=0}^{n_{col}(N+1)-1} C_k \left(\frac{d}{dr} S_k(r)\right) \\ \frac{d^2}{dr^2}\psi_\ell(r) &= \sum_{k=0}^{n_{col}(N+1)-1} C_k \left(\frac{d^2}{dr^2} S_k(r)\right) \end{aligned}$$

Collocation method

(2) We associate n_{col} local orthogonal polynomials of order $2n_{col}$ *-1* with each grid point:



$$\psi_\ell(r) = \sum_{k=0}^{n_{col}(N+1)-1} C_k S_k(r) = \sum_{k=n_{col}(i-1)}^{n_{col}(i+1)-1} C_k S_k(r) \quad if \quad r_{i-1} < r \le r_i$$

$$\frac{d^2}{dr^2}\psi_\ell(r) = \sum_{k=0}^{n_{col}(N+1)-1} C_k \left(\frac{d^2}{dr^2} S_k(r)\right) = \sum_{k=n_{col}(i-1)}^{n_{col}(i+1)-1} C_k \left(\frac{d^2}{dr^2} S_k(r)\right) \quad if \quad r_{i-1} < r \le r_i$$

(3) It can be demonstrated: that the solution will be the most accurate if diff. equation is satisfied on the n_{col} Gauss-quadrature points of each grids domain ($xg_1, xg_2, xg_3, xg_4, .., xg_{ncol*N}$)

$$\left(E + \frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} - \frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2} - V_\ell(r)\right)\psi_\ell(r) = 0 \quad \Rightarrow \quad \begin{bmatrix} h_{10} & h_{11} & h_{12} & h_{13} & 0 & 0 & 0 \\ h_{20} & h_{21} & h_{22} & h_{23} & 0 & 0 & 0 \\ 0 & 0 & h_{32} & h_{33} & h_{34} & h_{35} & 0 \\ 0 & 0 & h_{42} & h_{43} & h_{44} & h_{45} & 0 \\ 0 & 0 & 0 & 0 & \vdots & \vdots & \vdots \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \\ \vdots \\ \vdots \\ C_{ncol*(N+1)-1} \end{bmatrix}$$

$N_{col}N$ equations

$N_{col}(N+1)$ coefficients

Collocation method

(4) Missing n_{col} equations we get from boundary conditions

$$\left(E+\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}-\frac{\hbar^2}{2\mu}\frac{\ell(\ell+1)}{r^2}-V_\ell(r)\right)\psi_\ell(r)=0 \quad\Rightarrow\quad \underbrace{\begin{bmatrix} & & & & & & \\ h_{10} & h_{11} & h_{12} & h_{13} & 0 & 0 & 0 \\ h_{20} & h_{21} & h_{22} & h_{23} & 0 & 0 & 0 \\ 0 & 0 & h_{32} & h_{33} & h_{34} & h_{35} & 0 \\ 0 & 0 & h_{42} & h_{43} & h_{44} & h_{45} & 0 \\ 0 & 0 & 0 & 0 & \vdots & \vdots & \vdots \\ & & & & & & \end{bmatrix}}_{n_{col}N \text{ equations}} \underbrace{\begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ \vdots \\ \vdots \\ \vdots \\ C_{ncol*(N+1)-1} \end{bmatrix}}_{n_{col}(N+1) \text{ coefficients}}$$

- Gridstart point condition $\psi_\ell(0)=0 \quad\Rightarrow\quad C_0=0$

- Endpoint of the grid: n_{col}-1 conditions

a) Add n_{col}-1 equations from the boundary condition
(Easy for the bound state $\psi_\ell(r_{\max})=0 \quad\Rightarrow\quad C_{n_{col}N}=0$)

b) For the scattering use the trick: $C_{n_{col}N}=1$

(5) Remains to solve corresponding linear algebra problem

$[A]C^{(i)}=E^{(i)}C^{(i)}$ For bound states eigenvalue-eigenvector problem of size $n_{col}N * n_{col}N$

$[A]C=X$ For scattering states system of $n_{col}N$ linear equations

How to find eigenvalue-eigenvector (bound state) problem?

$$[A]C^{(i)} = E_{(i)}C^{(i)}$$

- Diagonalize by the existing linear algebra packages – getting all the eigenvalues (might be slow, not adapted to your problem)

But you often need only few negative eigenvalues

- Power method

$$|\psi\rangle_0 = \sum_i c_i^0 |\psi^{(i)}\rangle \quad with \quad \hat{H}|\psi^{(i)}\rangle = E^{(i)}|\psi^{(i)}\rangle$$

$$|\psi\rangle_1 = \hat{H}|\psi\rangle_0 = \hat{H}\sum_i c_i^0 |\psi^{(i)}\rangle = \sum_i E^{(i)} c_i^0 |\psi^{(i)}\rangle$$

$$\ldots$$

$$|\psi\rangle_n = \underbrace{\hat{H}\hat{H}....\hat{H}}_{n}\sum_i |\psi^{(i)}\rangle = \sum_i \left(E^{(i)}\right)^n c_i^0 |\psi^{(i)}\rangle \approx \left(E^{(j)}\right)^n c_i^0 |\psi^{(j)}\rangle$$

Largest eigenvalue

- Iteration inverse method

$$\left(\hat{H} - E_0\right)|\psi\rangle_1 = |\psi\rangle_0 \quad then \quad |\psi\rangle_1 = \left(\hat{H} - E_0\right)^{-1}|\psi\rangle_0 = \sum_i \frac{c_i^0}{E^{(i)} - E_0}|\psi^{(i)}\rangle$$

$$\left(\hat{H} - E_0\right)|\psi\rangle_2 = |\psi\rangle_1$$

$$\ldots$$

$$\left(\hat{H} - E_0\right)|\psi\rangle_n = |\psi\rangle_{n-1} \quad and \quad |\psi\rangle_n = \sum_i \frac{c_i^0}{\left(E^{(i)} - E_0\right)^n}|\psi^{(i)}\rangle \approx \frac{c_j^0}{\left(E^{(j)} - E_0\right)^n}|\psi^{(j)}\rangle$$

Eigenvalue closest to E_0

How to extract the phaseshifts? (scattering problem)

- Logarithmic derivative method

$$\tilde{\psi}_\ell(r_{big}) \approx c\left[\hat{j}_\ell(kr_{big}) + tg\delta_\ell(k)\hat{n}_\ell(kr_{big})\right]$$

$$\tilde{\psi}'_\ell(r_{big}) \approx ck\left[\hat{j}'_\ell(kr_{big}) + tg\delta_\ell(k)\hat{n}'_\ell(kr_{big})\right]$$

$$\Longrightarrow \quad tg\delta_\ell(k) \approx \frac{\hat{j}'_\ell(kr_{big}) - \hat{j}_\ell(kr_{big})\dfrac{\tilde{\psi}'_\ell(r_{big})}{k\tilde{\psi}_\ell(r_{big})}}{\hat{n}'_\ell(kr_{big}) - \hat{n}_\ell(kr_{big})\dfrac{\tilde{\psi}'_\ell(r_{big})}{k\tilde{\psi}_\ell(r_{big})}}$$

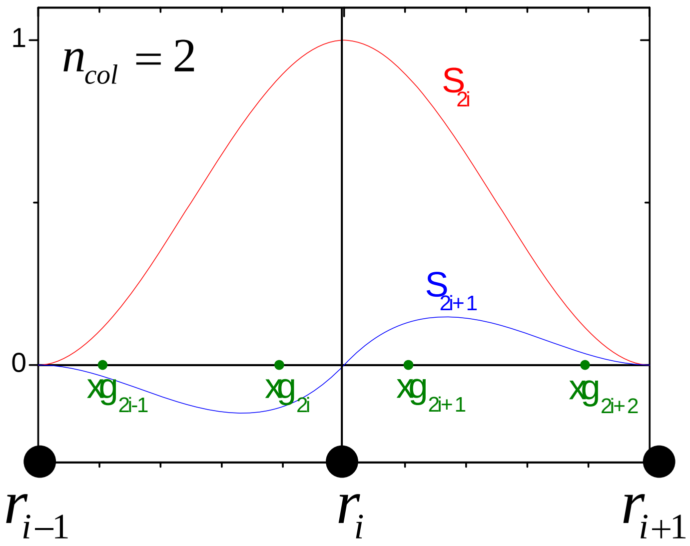
- Integral method

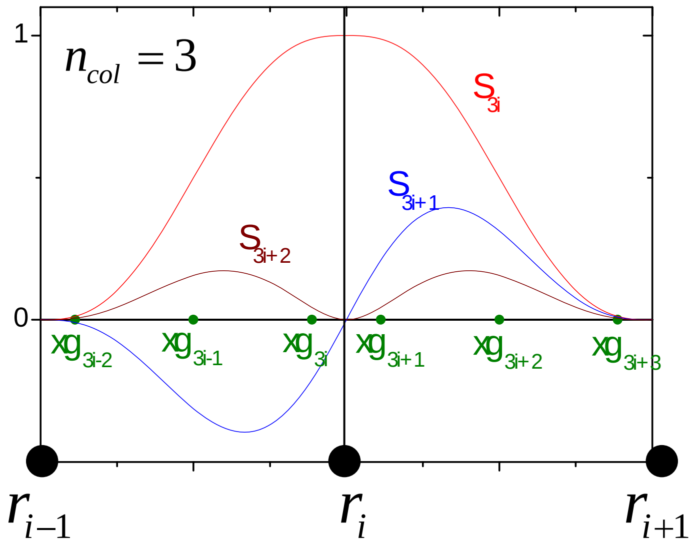
$$tg\delta_\ell(k) = -\frac{2\mu}{\hbar^2}k\int_0^\infty \hat{j}_\ell(kr)V(r)\psi_\ell(r)\,dr \approx -\frac{1}{c}\overbrace{\frac{2\mu}{\hbar^2}k\int_0^{r_{\max}} \hat{j}_\ell(kr)V(r)\tilde{\psi}_\ell(r)\,dr}^{I}$$

$$c \approx \frac{\tilde{\psi}_\ell(r_{\max})}{\hat{j}_\ell(kr_{\max}) + tg\delta_\ell(k)\hat{n}_\ell(kr_{\max})}$$

$$\Longrightarrow \quad tg\delta_\ell(k) \approx \frac{I\cdot\hat{j}_\ell(kr_{\max})}{\tilde{\psi}_\ell(r_{\max}) - I\cdot\hat{n}_\ell(kr_{\max})}$$

Expressions for cubic and quintic polynomials:





$forX_{i-1} \leq x \leq X_i$ $(withr = \frac{x-X_{i-1}}{X_i-X_{i-1}})$

$$\begin{cases} S_{2i}(x) = r^2(3-2r) \\ S_{2i+1}(x) = -(X_i - X_{i-1})r^2(1-r) \end{cases}$$

$forX_i \leq x \leq X_{i+1}$ $(withr = \frac{x-X_i}{X_{i+1}-X_i})$

$$\begin{cases} S_{2i}(x) = (1-r)^2(1+2r) \\ S_{2i+1}(x) = (X_{i+1} - X_i)r(1-r)^2 \end{cases}$$

$forX_{i-1} \leq x \leq X_i$ $(withr = \frac{x-X_{i-1}}{X_i-X_{i-1}})$

$$\begin{cases} S_{3i}(x) = r^3\left[3(1-r)(3-2r)+1\right] \\ S_{3i+1}(x) = -(X_i - X_{i-1})\left(1-r^3\right)(1+3r) \\ S_{3i+2}(x) = \frac{1}{2}(X_i - X_{i-1})^2 r^2 (1-r)^3 \end{cases}$$

$forX_i \leq x \leq X_{i+1}$ $(withr = \frac{x-X_i}{X_{i+1}-X_i})$

$$\begin{cases} S_{3i}(x) = \left(1-r^3\right)\left[1+3r(1+2r)\right] \\ S_{3i+1}(x) = (X_{i+1} - X_i)r^3(1-r)(4-3r) \\ S_{3i+2}(x) = \frac{1}{2}(X_i - X_{i-1})^2 r^3 (1-r)^2 \end{cases}$$