Numerov method
(exercise)

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Two-body Schrödinger equation

$$E\Psi(\boldsymbol{r}) = \left[-\frac{\hbar^2}{2\mu}\Delta + V(\boldsymbol{r})\right]\Psi(\boldsymbol{r})$$

where $\mu = m_1 m_2/(m_1 + m_2)$ is the reduce mass, $\boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2$, and $\Delta = \boldsymbol{\nabla}^2$

→ Assuming central potential $V(\boldsymbol{r}) = V(|\boldsymbol{r}|) = V(r)$ and introducing radial coordinates

$$E\Psi(r,\theta,\varphi) = \left[-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial r^2}r^2 + \frac{\boldsymbol{L}^2}{2\mu r^2} + V(r)\right]\Psi(r,\theta,\varphi)$$

→ Separating the wave function $\Psi(r,\theta,\varphi) = \frac{u_l(r)}{r}Y_{lm}(\theta,\varphi)$ (radial and angular part) and taking into account $\boldsymbol{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)\hbar Y_{lm}(\theta,\varphi)$

yields **RADIAL EQUATION**

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

Numerov method

→ we want to solve the **RADIAL EQUATION** numerically

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} u_l(r) + k(r) u_l(r) = 0, \qquad k(r) = \frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2\mu r^2}\right]$$

→ **TAYLOR EXPANSION** of $u_l(r) \equiv u(r)$

$$u_{n+1}(r) = u(r+h) = u_n(r) + h u_n^{(1)}(r) + \frac{h^2}{2} u_n^{(2)}(r) + \frac{h^3}{6} u_n^{(3)}(r) + \frac{h^4}{24} u_n^{(4)}(r) + \mathcal{O}(h^5)$$

$$u_{n-1}(r) = u(r-h) = u_n(r) - h u_n^{(1)}(r) + \frac{h^2}{2} u_n^{(2)}(r) - \frac{h^3}{6} u_n^{(3)}(r) + \frac{h^4}{24} u_n^{(4)}(r) - \mathcal{O}(h^5)$$

where $h << 1$ is the step size

→ summing Taylor expansions for $u_{n+1}(r)$ and $u_{n-1}(r)$

$$u_{n+1}(r) + u_{n-1}(r) = 2u_n(r) + h^2 u_n^{(2)}(r) + \frac{h^4}{12} u_n^{(4)}(r) + \mathcal{O}(h^6)$$

Numerov method

→ slightly rewriting the last expression on the previous slide

$$\begin{aligned} u_n^{(2)}(r) &= \frac{1}{h^2}\left[u_{n+1}(r) + u_{n-1}(r) - 2u_n(r) - \frac{h^4}{12}u_n^{(4)}(r) - \mathcal{O}(h^6)\right] \\ &= \frac{1}{h^2}\left[u_{n+1}(r) + u_{n-1}(r) - 2u_n(r)\right] - \frac{h^2}{12}u_n^{(4)}(r) - \mathcal{O}(h^4) \end{aligned}$$

we deal with the second derivative $u_n^{(2)}(r)$ and the fourth derivative $-\frac{h^2}{12}u_n^{(4)}(r)$ terms
→ using Schrödinger equation

$$\begin{aligned} u_n^{(2)}(r) &= -k_n(r)u_n(r) \\ -\frac{h^2}{12}u_n^{(4)}(r) &= -\frac{h^2}{12}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\left[u_n^{(2)}(r)\right] = \frac{h^2}{12}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\left[k_n(r)u_n(r)\right] \end{aligned}$$

and elementary difference formula

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}\left[k_n(r)u_n(r)\right] = \frac{1}{h^2}\left[k_{n+1}(r)u_{n+1}(r) + k_{n-1}(r)u_{n-1}(r) - 2k_n(r)u_n(r)\right]$$

Numerov method

$$-k_n(r)u_n(r) = \frac{1}{h^2}\left[u_{n+1}(r) + u_{n-1}(r) - 2u_n(r)\right] + \frac{1}{12}\left[k_{n+1}(r)u_{n+1}(r) + k_{n-1}(r)u_{n-1}(r) - 2k_n(r)u_n(r)\right] - \mathcal{O}(h^4)$$

multiplying by h^2

$$-h^2 k_n(r)u_n(r) = u_{n+1}(r) + u_{n-1}(r) - 2u_n(r) + \frac{h^2}{12}\left[k_{n+1}(r)u_{n+1}(r) + k_{n-1}(r)u_{n-1}(r) - 2k_n(r)u_n(r)\right] - \mathcal{O}(h^6)$$

we obtain recursive relation for $u_{n+1}(r)$ (Numerov)

$$u_{n+1}(r) = \frac{2\left[1 - \frac{5}{12}h^2 k_n(r)\right]u_n(r) - \left[1 + \frac{1}{12}h^2 k_{n-1}(r)\right]u_{n-1}(r)}{1 + \frac{h^2}{12}k_{n+1}(r)} + \mathcal{O}(h^6)$$

$\rightarrow$ erron in one step is $\mathcal{O}(h^6)$; errors can add up (global uncertanties) $\mathcal{O}(h^5)$
[Numerov is 5th order method]

Behavior of $u_l(r)$ close to the origin

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

→ if $V(r)$ approches zero slower than $1/r^2$ the centrifugal barrier dominates

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_l(r) \approx \frac{l(l+1)}{r^2}u_l(r)$$

→ using ansatz $u_l(r) \sim r^\alpha$ we find $u(r) \approx Ar^{l+1} + Br^{-l}$
→ $\Psi(\boldsymbol{r})$ should be normalizable, this means that $u_l(r)/r$ should be square integrable close to $r = 0$

$$\int_a^b \left(\frac{r^\alpha}{r}\right)^2 r^2 \mathrm{d}r = \int_a^b r^{2\alpha}\mathrm{d}r = \frac{1}{2\alpha}\left[b^{2\alpha+1} - a^{2\alpha+1}\right]$$

→ for $\alpha < -1/2$ diverges as $a \to 0$, consequently, we reject r^{-l} solution

$$u_l(r \to 0) \approx r^{l+1}$$

→ for Numerov we can set $u_0 = 0$ and $u_1 = h^{l+1}$

Bound state calculations via Numerov method

→ Numerov method needs initial conditions u_0, u_1, and the energy E

→ for bound states the energy E is usually the observable we aim to calculate ...

How do we proceed ?

For $r > r_{\max}$ we obtain Schrödinger equation in a form :

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} u_l(r) \simeq \kappa^2 u_l(r), \qquad \kappa^2 = -\frac{2\mu}{\hbar^2} E$$

with solution $u_l(r) = Ae^{-\kappa r} + Be^{\kappa r}$

→ for bound states $E < 0$, $\kappa > 0$ and due to the normalization condition

$$u_l(r > r_{\max}) \simeq Ae^{-\sqrt{2\mu|E|/\hbar^2}r}$$

Algorithm :

We choose an energy interval $\langle E_{\min}; E_{\max}\rangle$; inside this interval we search for such E for which Numerov solution at $r > r_{\max}$ yields $u_l(r) = 0$.

Phase shift calculation via Numerov method

INTERANL region ($r < r_{\max}$) :

$$\frac{\mathrm{d}^2}{\mathrm{d}r^2} u_l^{(\mathrm{int})}(r) = -\frac{2\mu}{\hbar^2}\left[E - V(r) - \frac{\hbar^2 l(l+1)}{2\mu r^2}\right] u_l^{(\mathrm{int})}(r), \qquad E = \frac{k^2}{(2\mu)}$$

$\rightarrow$ Numerov method for $E > 0$

EXTERNAL region ($r > r_{\max}$) :

$$u_l^{(\mathrm{ext})}(r) = A\left[\cos(\delta)\ kr\ j_l(kr) - \sin(\delta)\ kr\ n_l(kr)\right]$$

Using Numerov solution at $r_1, r_2 > r_{\max}$:

$$\frac{u_l^{(\mathrm{int})}(r_1)}{u_l^{(\mathrm{int})}(r_2)} = \frac{u_l^{(\mathrm{ext})}(r_1)}{u_l^{(\mathrm{ext})}(r_2)} \quad \longrightarrow \quad \tan(\delta) = \frac{\beta j_l(kr_1) - j_l(kr_2)}{\beta n_l(kr_1) - n_l(kr_2)}, \qquad \beta = \frac{r_1 u_l^{(\mathrm{int})}(r_2)}{r_2 u_l^{(\mathrm{int})}(r_1)}$$

Phase shift calculation via Numerov method

Using Logarithmic derivative at $r_1 > r_{\max}$:

$$\frac{\left(u_l^{(\mathrm{int})}(r_1)\right)'}{u_l^{(\mathrm{int})}(r_1)} = \frac{\left(u_l^{(\mathrm{ext})}(r_1)\right)'}{u_l^{(\mathrm{ext})}(r_1)} \quad \longrightarrow \quad \tan(\delta) = \frac{\beta j_l(kr_1) - j_l(kr_2)}{\beta n_l(kr_1) - n_l(kr_2)}, \qquad \beta = \frac{r_1 u_l^{(\mathrm{int})}(r_2)}{r_2 u_l^{(\mathrm{int})}(r_1)}$$