Compute wave functions in multichannel collisions with non-local potentials using the R-matrix method

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Previous project:
A program to compute wave functions of neutrons and protons in nuclear scattering problems involving **non-local potentials**
Research Question

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Extend this project to account for multiple channels.
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\[
\left[ -\frac{\hbar^2}{2\mu_c} \left( \frac{d^2}{dr^2} - \frac{l_c(l_c+1)}{r^2} \right) + V_c(r) + E_c - E \right] u_{c(c_0)}(r) + \sum_{c'} \int_0^\infty V_{cc'}(r, r') u_{c'(c_0)}(r') dr' = 0 \quad (1)
\]
Motivation

- Wave functions are ubiquitous in theoretical nuclear physics
  - There is a demand for fast algorithms to compute complicated wave functions

\[ V_{nl}^{u}(r) = \int_{0}^{\infty} V(r, r') u(r') \, dr' \] (2)

During collisions, nuclei can enter multiple channels, or states.
- To account for these, we must introduce coupling into our potential
  \[ V^{ uc}(r) = \sum c' V_{cc'}^{u}(r) u_{c'}(r) \] (3)
Motivation

- Wave functions are ubiquitous in theoretical nuclear physics
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- Nuclear potentials are **non-local**, meaning the force on a particle at one location depends on the force on it at all other locations

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  \]  
  (2)
- During collisions, nuclei can enter multiple **channels**, or states.
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    \[
    V(r)u_c(r) = \sum_{c'} V_{cc'}(r)u_{c'}(r)
    \]  
    (3)
Motivation

large $k$ - e.g. nucleus-nucleus

$$R_P, k, L$$

$$b$$

$$R_T$$

$$|S_L|$$

absorption

transmission

$$k(R_P + R_T)$$
The R-matrix method

First, divide the problem into two regions, internal and external, at the channel radius, $a$

- We ignore nuclear forces in the external region so that $u^{\text{ext}}(r)$ is solved analytically

\[ \sum_{c} c' \left( T_{c} + L_{c} + E_{c} - E_{c'} \right) \delta_{cc'} + V_{cc'} u^{\text{int}}_{c'} (\text{Bloch-Schrodinger Eq.}) \]
The R-matrix method

First, divide the problem into two regions, internal and external, at the channel radius, $a$

- We ignore nuclear forces in the external region so that $u^{\text{ext}}(r)$ is solved analytically

- We then relate $u^{\text{int}}(r)$ with $u^{\text{ext}}(r)$

$$
\sum_{c'\prime} [(T_c + \mathcal{L}_c + E_c - E)\delta_{cc'} + V_{cc'}] u^{\text{int}}_{c'\prime} = \mathcal{L}_c u^{\text{ext}}_c
$$

(Bloch-Schrodinger Eq.)

---

The R-matrix method

- We expand the wave function over a finite basis

\[ u_c^{\text{int}}(r) = \sum_{j=1}^{N} c_j \varphi_j(r) \]  

(4)
The R-matrix method

- We expand the wave function over a finite basis

\[ u^{\text{int}}_c(r) = \sum_{j=1}^{N} c_j \varphi_j(r) \]  

(4)

- The problem is reduced to matrix calculations

\[ R_{cc'}(E) = \frac{\hbar^2}{2\sqrt{\mu_c\mu_{c'}} a} \sum_{i,i'=1}^{N} \varphi_i(a)(C^{-1})_{ci,c'i'}\varphi_i(a) \]  

(5)

\[ C_{ci,c'i'} = \langle \varphi_i | T_c + L_c + E_c - E | \varphi_{i'} \rangle \delta_{cc'} + \langle \varphi_i | V_{cc'} | \varphi_{i'} \rangle \]  

(6)
The Lagrange basis

Lagrange functions:

\[ \varphi_i(r) = (-1)^{N+i} \left( \frac{r}{\alpha x_i} \right) \sqrt{\alpha x_i (1 - x_i)} \frac{P_N(2r/a - 1)}{r - \alpha x_i} \]  

(7)

where \( x_i \) are the roots of \( P_N(2x - 1) \)

From the Gauss-Legendre quadrature rule:

\[ \langle \varphi_i | \varphi_j \rangle = \int_0^a \varphi_i(r) \varphi_j(r) dr \approx \delta_{ij} \]  

(8)

\[ \langle \varphi_i | V(r) | \varphi_j \rangle \approx V(ax_i) \delta_{ij} \]  

(9)

\[ \langle \varphi_i | W(r, r') | \varphi_j \rangle \approx a \sqrt{\lambda_i \lambda_j} W(ax_i, ax_j) \]  

(10)
Program structure (C++)

Channel
+ E, l, j, m, mu, B : double
+ CoulombFunctions(radius, energy)
+ CentrifugalPotential(radius)

LagrangeBasis
+ weights[]
+ abcissae[]
+ LagrangeFunction(i, radius)

System
+ Channel radius, Energy : double
+ C, R, U : matrix
- Target, Projectile : Particle
- Channels : Channel[]
- Local, Nonlocal : OpticalPotential
- Basis : LagrangeBasis
+ WaveFunctions(output file)

Particle
+ Protons
+ Neutrons

OpticalPotential
+ V : Volume Potential
+ D : Surface Potential
+ SO : Spin Orbit Potential
+ TotalPotential(radius)

NonLocalOpticalPotential
+ Range of nonlocality : double
+ TotalPotential(radius)

Potential
+ V, r, a
+ getValue(radius)

VolumePotential

SpinOrbitPotential

SurfacePotential
(a) $n^{+10}$Be elastic scattering at 10 MeV overlaid with expected results for single channel case.

(b) $n^{+10}$Be elastic scattering at 10 MeV output including $I = 0^+$ and $I = 2^+$ ($E_c = 3.368$ MeV) channels
Results

(a) Plot showing convergence to accurate results with number of Lagrange functions in basis expansion

(b) Time analysis showing $10^3$ speedup from original program (Python)
Advantages, Limitations, & Future work

Advantages
- Fast program, accounts for arbitrary number of channels, MPI implementation

Limitations
- Current bug with normalization
- Does not handle closed channels

Future work
- Applying the program in Uncertainty Quantification problems
- Using the program to fit predictions to experimental data
Acknowledgements

Advanced Computational Research Experience for Students
\[ L_c = \frac{\hbar^2}{2\mu_c} \delta(r - a) \left( \frac{d}{dr} - \frac{B_c}{r} \right) \]  
(Bloch operator)

\[ u_c(a) = \sum_{c'} \sqrt{\frac{\mu_c}{\mu_{c'}}} R_{cc'} [au_{c'}(a) - B_{c'} u_{c'}(a)] \]  
(R-matrix)