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

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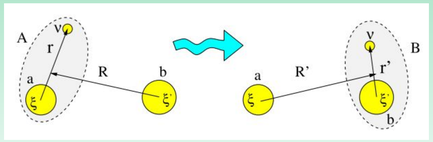
Motivation

To describe quantum properties and predict the positions of particles after collisions, we use wave functions. The wave functions for two-body nuclear collisions are also important input to understand more complicated three-body collisions, specifically nuclear transfer reactions [2].

Previous solutions to this problem have been computationally time-consuming.
Since wave functions appear often in nuclear physics, there is a demand for faster methods for calculating them.



Nuclear potentials in reality are *nonlocal*, meaning the nuclear force on a particle at one point depends on the force on that particle at all other points.
Most problems also involve multiple states, or *channels*. This introduces coupling into the equations.

Theory [1]

$$\left[-\frac{\hbar^2}{2\mu_c}\left(\frac{d^2}{dr^2}-\frac{l_c(l_c+1)}{r^2}\right)+V_c(r)+E_c-E\right]u_{c(c_0)}(r)+\sum_{c'}\int_0^\infty V_{cc'}(r,r')u_{c'(c_0)}(r')dr'=0$$

The R-matrix method makes use of the assumption that nuclear forces are short-ranged. The problem is divided into two regions, internal and external, which are separated at the channel radius *a*. Nuclear forces are only considered in the internal region so that the wave function in the external region is calculated analytically.

$$\mathcal{L}_c(B)=\frac{\hbar^2}{2\mu_c}\delta(r-a)\left(\frac{d}{dr}-\frac{B_c}{r}\right)$$

First, we introduce the Bloch surface operator into the Schrödinger equation to relate the internal and external wave functions

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

$$u_c^{int}(r)=\sum_{j=1}^{N}c_{cj}\varphi_j(r)$$

Next, we expand the partial wave functions over a finite basis (see Lagrange Mesh section)

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

$$C_{ci,c'i'}=\langle\varphi_i|T_c+\mathcal{L}_c+E_c-E|\varphi_{i'}\rangle\,\delta_{cc'}+\langle\varphi_i|V_{cc'}|\varphi_{i'}\rangle$$

$$u_{c(c_0)}^{int}(r)=\sum_{c'}\mathcal{L}_{c'}u_{c'(c_0)}^{ext}(a)\sum_{i,i'=1}^{N}\varphi_i(r)(C^{-1})_{ci,c'i'}\varphi_{i'}(a)$$

By taking the operators from the Schrödinger equation on the basis functions, we calculate the R-matrix, which is used to compute the external wave functions. We can then compute the internal wave functions at all points.

Lagrange Mesh

For the finite basis expansion required by the R-matrix method, we use the Lagrange functions defined here:

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

Due to the Gauss-Legendre quadrature rule, when evaluating the potentials on these functions, one only has to consider the value of the potentials at the mesh points, ax_i
This makes the R-matrix method **much faster** than other techniques which use direct integration [3].

Gauss quadrature rules:

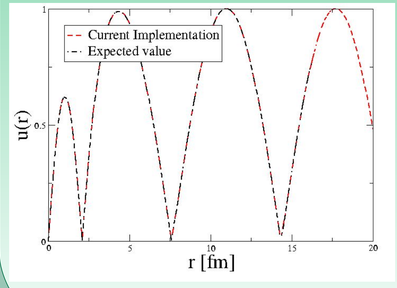
$$\langle\varphi_i|\varphi_j\rangle=\int_0^a\varphi_i(r)\varphi_j(r)dr\approx\delta_{ij}$$

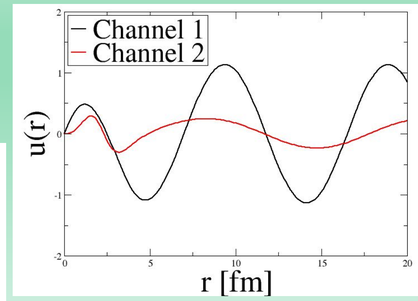
$$\langle\varphi_i|V(r)|\varphi_j\rangle\approx V(ax_i)\delta_{ij}$$

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

Results

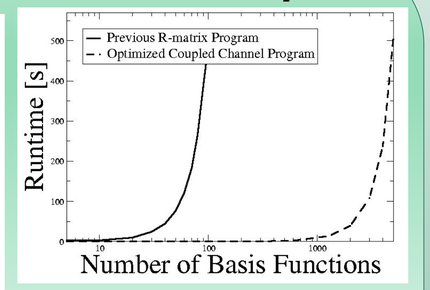
(below) Elastic scattering partial wave function for n+^{10}Be at E=10 MeV, potential parameters from [4]. Absolute value overlaid with output of code from [1].





(above) n+^{10}Be at E=10 MeV with potential parameters from [4]. Coupling of the entrance channel (1) with the excitation channel (2) can be observed.

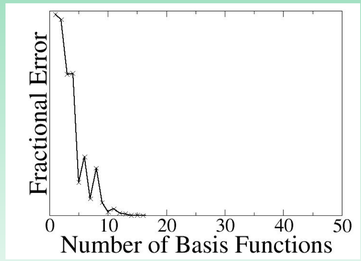
Runtime analysis



Improvement of the order of **~10^3** times from another implementation.
Speed up partially due to the Armadillo C++ library [5] used for the matrix calculations.
Matrix Inversion is the most time consuming step at high precision.

Convergence with Number of Basis Functions

Fractional error of the modulus of the wavefunction at R=1.20 fm including N Lagrange functions and the results obtained for N=300

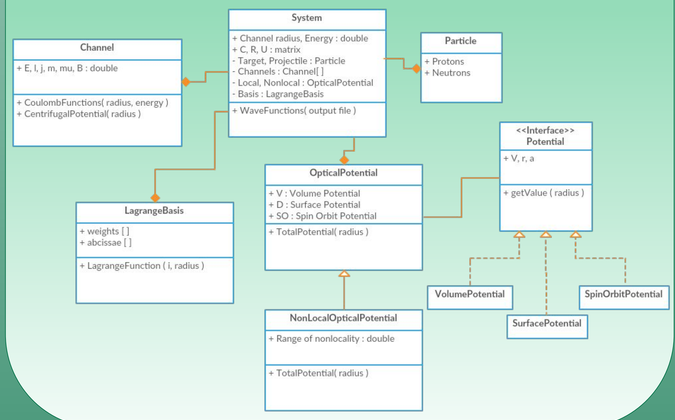


n-^{10}Be at E=10 MeV

Convergence is obtained at **N=15**.

Code Design

The program was written in C++ using Object-Oriented Programming techniques to increase modularity. An input file format was designed to make the program user-friendly.



Advantages of the code

- 10^3 times faster the predecessor code
- Handles an arbitrary number of channels
- Modular structure for easier future extensions
- Includes parallel processing (MPI)

Future Research

There are many promising continuations to this research in R-matrix theory, including:

- Applying the program to compute wave functions in cases with many channels with High
- Extending the current implementation to include closed channels
- Using the program to fit predictions to experimental data
- Extending the R-matrix theory to three-body collisions
- Exploring Quantum Computing algorithms for the R-matrix method

References

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