

The two-nucleon and three-nucleon system in three dimensions

Kacper Topolnicki

23 września 2014



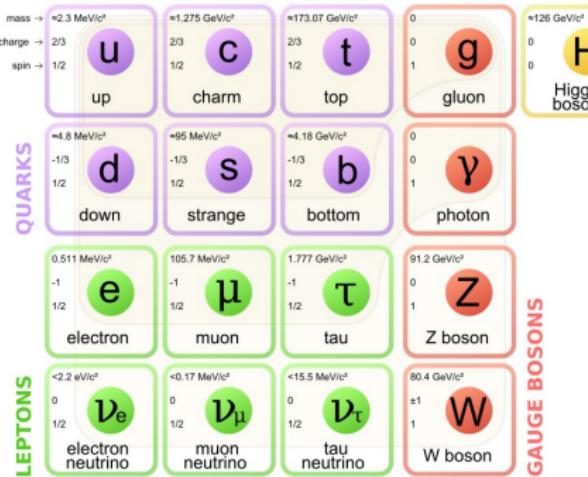
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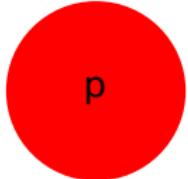
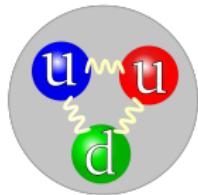


THE STANDARD MODEL OF PARTICLE PHYSICS

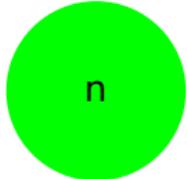
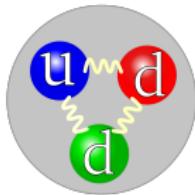


"Standard Model of Elementary Particles" by MissMJ - Own work by uploader, PBS NOVA [1], Fermilab, Office of Science, United States Department of Energy, Particle Data Group. Licensed under Creative Commons Attribution 3.0 via Wikimedia Commons - http://commons.wikimedia.org/wiki/File:Standard_Model_of_Elementary_Particles.svg#mediaviewer/File:Standard_Model_of_Elementary_Particles.svg

LOW ENERGIES

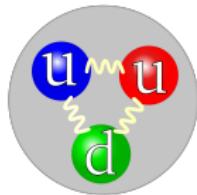


- In order to gain a better understanding of the theory the low energy sector needs to be studied
- The everyday world is composed mainly from low energy protons and neutrons
- Effective, coulomb like, models of nuclear interactions are introduced

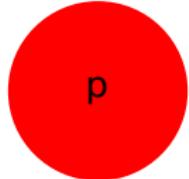
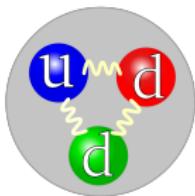


OUR GOAL: Create tools to verify modern nuclear potentials constructed from effective field theory.

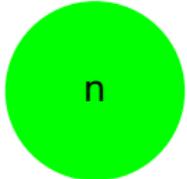
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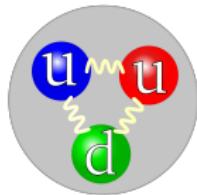
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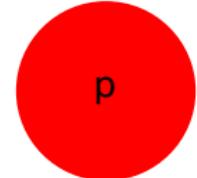
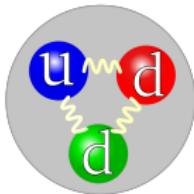
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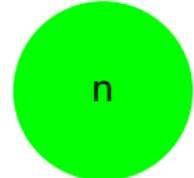
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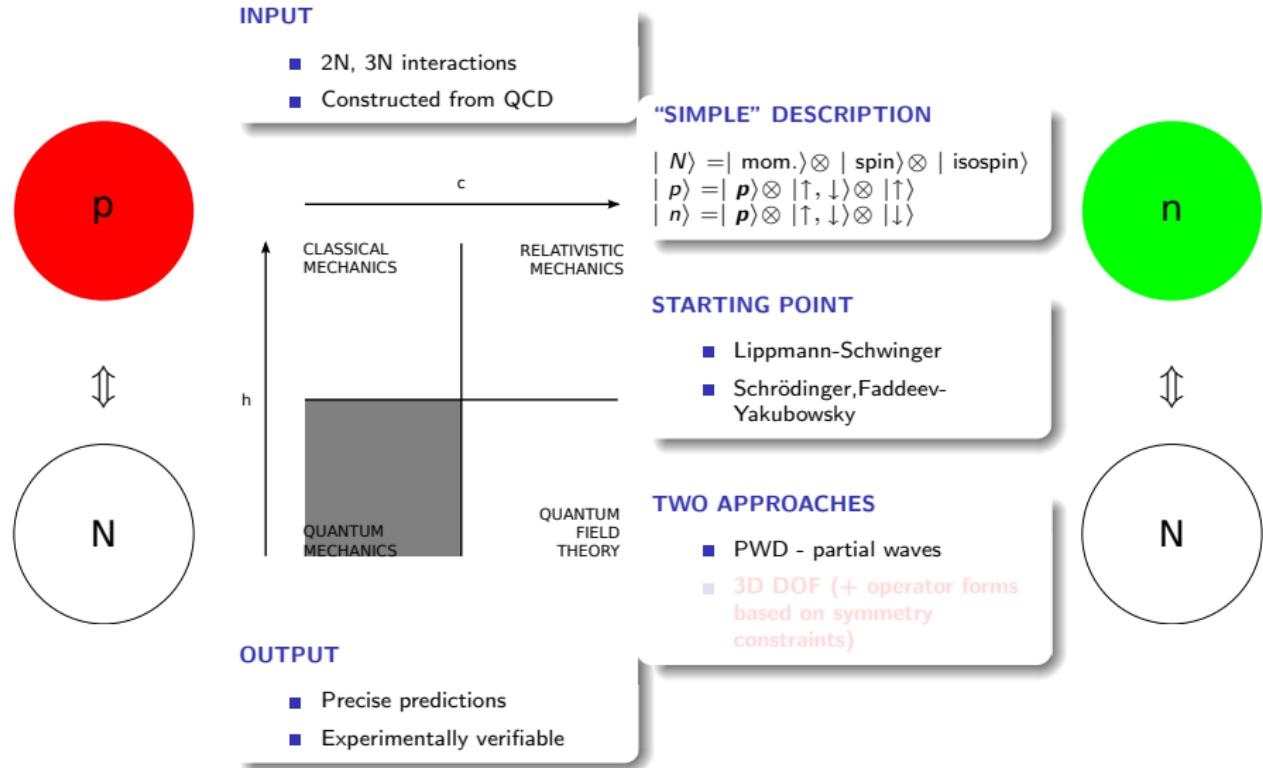
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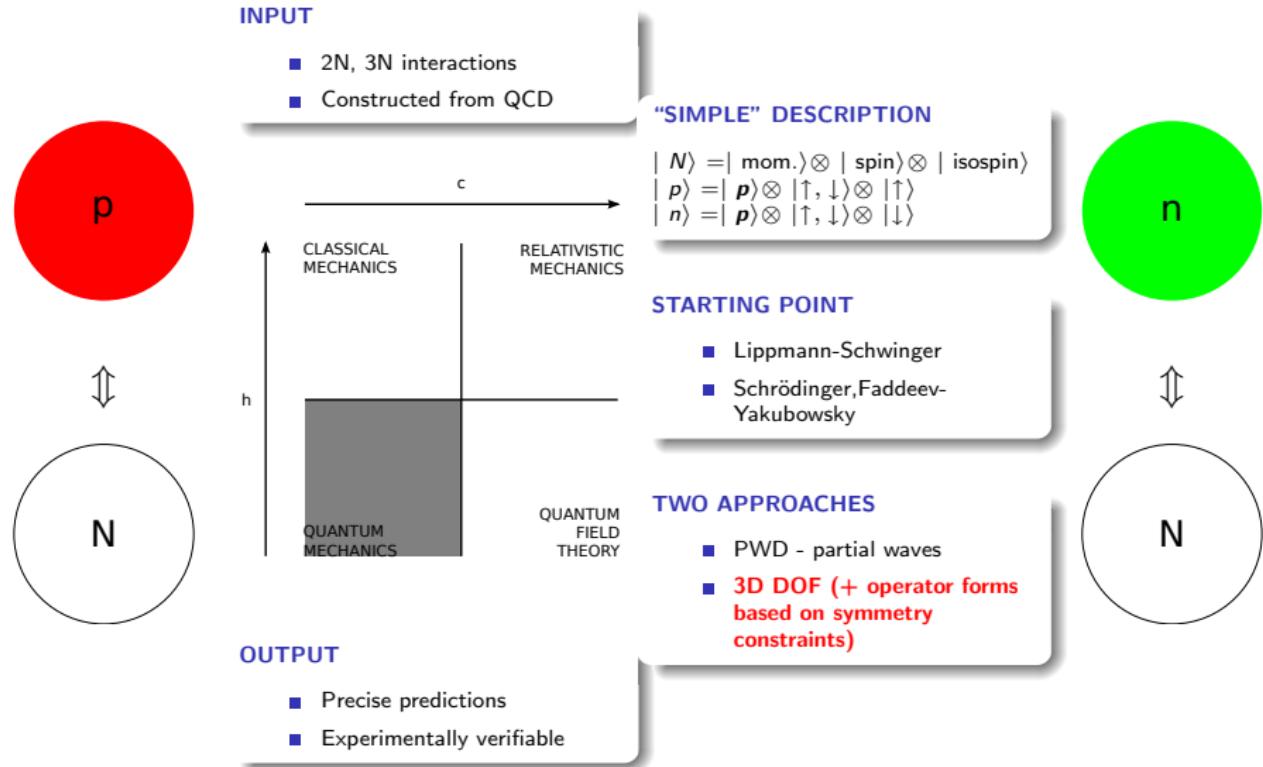
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DESCRIPTION



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- Two body potential:

- $V(1, 2) + V(2, 3) + V(3, 1)$
- $V(i, j)$ function of the degrees of freedom of particles i, j
- solar system (gravity)
- classical electrostatic interactions

- Three body potential:

- $V(1, 2) + V(2, 3) + V(3, 1) + V(3; 1, 2) + V(1; 2, 3) + V(2; 3, 1)$
- can not be expressed in terms of two body interactions
- $V(i; j, k)$ symmetric with respect to the exchange of particles j, k

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PROBLEMS

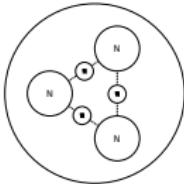
PRECISE CALCULATIONS

- Development of tools allowing for an easy incorporation of new models of 2N, 3N forces.
- 2N bound state (three dimensional formalism):

Two-nucleon systems in three dimensions
J. Golak, W. Glöckle, R. Skibiński, H. Witała, D. Rozpedzik, K. Topolnicki, I. Fachruddin, Ch. Elster and A. Nogga

Physical Review C 81(3):034006

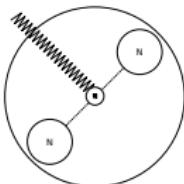
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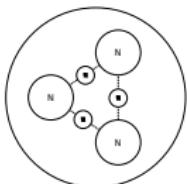

- ³H (different schemes)
- planned - ³He, 3N system resonances

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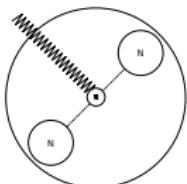


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Few-Body Systems 54(12):2427-2446

2013

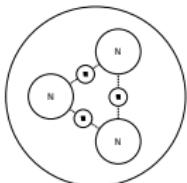
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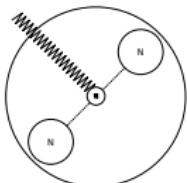


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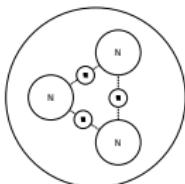
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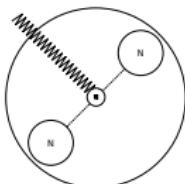


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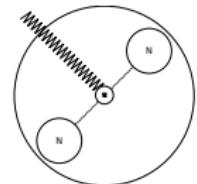
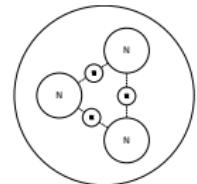
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Few-Body Systems 53(3-4):237-252

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- planned - 3N: eg. N-deuteron (under construction)



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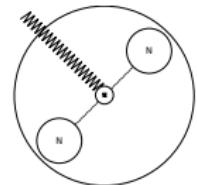
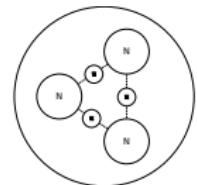
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Deuteron Disintegration in Three Dimensions

K. Topolnicki, J. Golak, R. Skibiński, A.E. Elmeshneb, W. Glöckle, A. Nogga and H. Kamada

Few-Body Systems 54(12):2233-2253

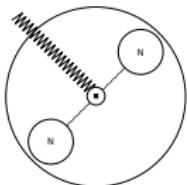
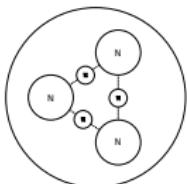
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Break-up channels in muon capture on ${}^3\text{He}$

J. Golak, R. Skibiński, H. Witała, K. Topolnicki, A.E. Elmeshneb, H. Kamada, A. Nogga and L.E. Marcucci

Phys. Rev. C 90(2):024001

2014



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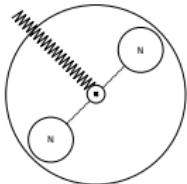
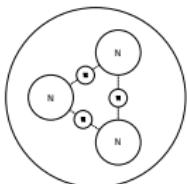
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A new way to perform partial-wave decompositions of few-nucleon forces

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The European Physical Journal A 43(2):241-250

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The European Physical Journal A 47(4):1-16

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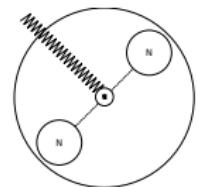
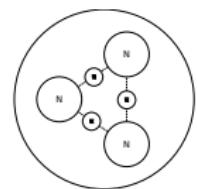
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- 2N, 3N forces, electro-weak currents including meson exchange
- Flexible calculation scheme, the possibility to quickly test new models
- planned - 4N forces, . . . , new models



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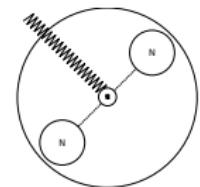
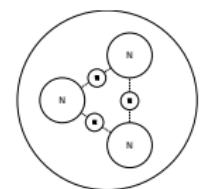
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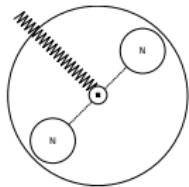
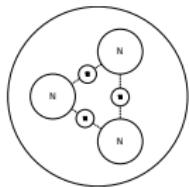
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FOUNDATIONS



THE FOUNDATIONS OF OUR CALCULATIONS

- 2N, 3N potentials:
 - traditional "realistic" nuclear interactions
 - chiral effective field theories inspired by QCD
- Electro-weak currents:
 - derived using the potentials
 - single nucleon and two nucleon operators

SYMBOLIC PROGRAMMING

CHALLENGE

- Solve the fundamental equations, without simplifications
- The expressions look good on paper . . . until you try to use a specific (2N,3N) force or (EM, weak) current model
- A very complicated numerical realization of seemingly simple matrix elements, for example:

$$\langle \Psi_{^3\text{H}} | j_{\text{weak}} | \Psi_{^3\text{He}} \rangle$$



SYMBOLIC PROGRAMMING

CHELLANGE

- Automatic code production is necessary:



How we invert Eqs. (26), (27) and (28) into Eq. (29) and obtain

$$\begin{aligned} & \sum_{i=1}^n \frac{1}{E - E_i - \omega_i t} \int d\lambda' \sqrt{\lambda'} \sum_{j=1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \\ & + \frac{1}{E - E_1 - \omega_1 t} \int d\lambda' \sqrt{\lambda'} \sum_{j=1}^n \left(C_{1j}^1(E_1, \lambda_1, \omega_1) C_{1j}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{1j}^2(E_1, \lambda_1, \omega_1) C_{1j}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \frac{1}{E - E_2 - \omega_2 t} \sum_{j=1}^n \int d\lambda' \sqrt{\lambda'} \sum_{i=1}^{j-1} \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \frac{1}{E - E_i - \omega_i t} \int d\lambda' \sqrt{\lambda'} \sum_{j=i+1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \left(\sum_{j=1}^n C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \left(\sum_{j=1}^n C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \\ & + \frac{1}{E - E_1 - \omega_1 t} \sum_{j=1}^n \int d\lambda' \sqrt{\lambda'} \sum_{i=1}^{j-1} \left(C_{ij}^1(E_1, \lambda_1, \omega_1) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_1, \lambda_1, \omega_1) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \int d\lambda' \sqrt{\lambda'} \sum_{j=i+1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \frac{1}{E - E_2 - \omega_2 t} \sum_{j=1}^n \int d\lambda' \sqrt{\lambda'} \sum_{i=1}^{j-1} \left(C_{ij}^1(E_2, \lambda_2, \omega_2) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_2, \lambda_2, \omega_2) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \int d\lambda' \sqrt{\lambda'} \sum_{j=i+1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \end{aligned}$$

This can be further simplified by noting

$$P_1 P_2 \dots P_n M_{11} M_{21} \dots M_{n1} = -\frac{1}{2} (M_{11} M_{21} \dots M_{n1}) + M_{11} M_{21} \dots M_{n1} = 0$$

which turns Eq. (29) into

$$\begin{aligned} & \sum_{i=1}^n \frac{1}{E - E_i - \omega_i t} \int d\lambda' \sqrt{\lambda'} \sum_{j=1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \\ & + \frac{1}{E - E_1 - \omega_1 t} \int d\lambda' \sqrt{\lambda'} \sum_{j=1}^n \left(C_{1j}^1(E_1, \lambda_1, \omega_1) C_{1j}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{1j}^2(E_1, \lambda_1, \omega_1) C_{1j}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \int d\lambda' \sqrt{\lambda'} \sum_{j=i+1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right. \\ & \quad \left. + C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \right) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \\ & + \sum_{i=1}^n \mu_i \sum_{j=1}^n \lambda_j C_{ij}^2(E_i, \lambda_i, \omega_i) C_{ij}^1(E_j, \lambda_j, \omega_j) \end{aligned}$$

Analogue to Eq. (27) in case of the derivative we now proceed from the left with $\frac{d}{dt} \int d\lambda' \sqrt{\lambda'} \sum_{j=1}^n \left(C_{ij}^1(E_i, \lambda_i, \omega_i) C_{ij}^2(E_j, \lambda_j, \omega_j) \right)$ and make even ... This leads to the following relations, which are all similar

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SYMBOLIC PROGRAMMING

CHELLANGE

- Automatic code production is necessary:
 - the numerical realization requires the creation of \approx 10000 lines of code implementing eg. potentials, currents etc.
 - carrying out this work by hand, for a single model, would take \approx 1 PhD
 - fixing bugs in the implementation is another \approx 3, 4 years :(
 - currently, with our newly developed tools, this work takes only a couple of hours :)



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SYMBOLIC PROGRAMMING



SOLUTION

- Development of tools for dealing with 2N and 3N systems with the use of symbolic programming (Mathematica®):
 - the ability to quickly adapt the calculations to new models of 2N, 3N forces, currents
 - a FORTRAN implementation is created automatically, the resulting code is ready to be compiled and linked to our code
 - we have a very universal tool but are only beginning to discover its possibilities

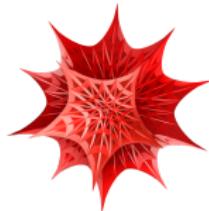


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NUMERICAL REALISATION

CHALLENGE

- We use symmetry considerations to limit the form of operators involved in the calculations. This leads to a reduction of the size of the numerical work.
- Some calculations are still, numerically, very heavy (3N bound state, the continuum of scattering states)
- Mainly large eigen-problems ($\propto 1000000 \times 1000000$)



NUMERICAL REALISATION

SOLUTION

- Krylov methods, Arnoldi iterations:
 - the possibility to turn the 1000000×1000000 dimensional problem to a smaller $\approx 100 \times 100$ problem
 - the iterations in our algorithms are still very demanding numerically
- We use large computing clusters. Access through LEN-PIC:
 - JUROPA, Jülich Supercomputing Center, Germany
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MY PLANS FOR THE NEAREST FUTURE:

- Further use of our tools
 - Extend calculations to include the description of 3N scattering
 - Electro-weak processes
 - Extend current calculations to 3He bound state with the Coulomb interaction
- Optimize the 3D calculations
- Test new models

THANK YOU FOR YOUR ATTENTION