AB INITIO STRUCTURE AND REACTIONS OF LIGHT NUCLEI

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INTRODUCTION

Structure of exotic nuclei

Ab initio structure and reactions

Fusion based energy generation

Nuclear astrophysics

Materials science
Nuclear astrophysics community relies on accurate fusion reaction observables among others.

Challenging for both experiment and theory:

- Low rates: due to Coulomb repulsion between target/projectile and low-energy reactions (quantum tunneling effects).
- Projectile and target are not fully ionized in a lab. This leads to laboratory electron screening.
- Fundamental theory is still missing.
Chiral effective field theory is a low-energy expansion of the interaction between nucleons with an estimation of the model uncertainties. Constrained to provide an accurate description of the A=2 and A=3 systems. Yet uncompleted… Predictions for nuclear structure and dynamic (A>3).
In configuration interaction methods we need to soften interaction to address the hard core. We use the Similarity-Renormalization-Group (SRG) method.

\[ H_\lambda = U_\lambda H U_\lambda^\dagger \]

\[ \frac{dH_\lambda}{d\lambda} = [\eta(\lambda), H_\lambda] \]

Unitary transformation

Flow parameter

Bare potential

Evolution with flow parameter \( \lambda \)

Evolved potential

- Preserves the physics
- Decouples high and low momentum
- Induces many-body forces
Methods develop in this presentation to solve the many body problem

\[
\Psi^{(A)}_{NCSM} = |A\lambda J^\pi T\rangle = \sum_\alpha c_\alpha |A\alpha j^z_\pi t_z\rangle
\]

Mixing coefficients (unknown)

A-body harmonic oscillator states

\[
|A\lambda J^\pi T\rangle_{SD} \phi_{00} (R^A_{c.m.})
\]

Second quantization

Can address bound and low-lying resonances (short range correlations)

\[
\Psi^{(A)}_{NCSM} = \sum_\lambda c_\lambda |A\lambda J^\pi T\rangle
\]

No-Core Shell Model

\[N_{\text{max}} \approx e^{-\alpha r}\]

• Methods develop in this presentation to solve the many body problem

\[ \Psi_{NCSM}^{(A)} = |A\lambda J^{\pi}T\rangle = \sum_{\alpha} c_{\alpha} |A\alpha j_{z}^{\pi}t_{z}\rangle \]

- Mixing coefficients (unknown)
- A-body harmonic oscillator states
- Second quantization

\[ |A\lambda J^{\pi}T\rangle_{SD} \Phi_{00}(\vec{R}_{c.m.}^{A}) \]

\[ \Psi_{RGM}^{(A)} = \sum_{v} \int d\vec{r} \; g_{v}(\vec{r}) \hat{A}_{v} \Phi_{v\vec{r}}^{(A-a,a)} \]

- Relative wave function (unknown)
- Antisymmetrizer
- Channel basis
- Cluster expansion technique

\[ \Psi_{NCSMC}^{(A)} = \sum_{\lambda} c_{\lambda} |A\lambda J^{\pi}T\rangle + \sum_{v} \int d\vec{r} \; g_{v}(\vec{r}) \hat{A}_{v} \Phi_{v\vec{r}}^{(A-a,a)} \]

Can address bound and low-lying resonances (short range correlations)

NCSM/RGM
Cluster formalism for elastic/inelastic
• Methods develop in this presentation to solve the many body problem

\[ \Psi^{(A)}_{NCSM} = |A\lambda J^\pi T\rangle = \sum_\alpha c_\alpha |A\alpha j_z^\pi t_z\rangle \]

Mixing coefficients (unknown)

A-body harmonic oscillator states

\[ |A\lambda J^\pi T\rangle_{SD} \phi_{00}(\vec{R}_{c.m.}^{A}) \]

Second quantization

Can address bound and low-lying resonances (short range correlations)

• The many body quantum problem is best described by the superposition of both type of wave functions

\[ \Psi^{(A)}_{NCSMC} = \sum_\lambda c_\lambda |A\lambda J^\pi T\rangle + \sum_v \int d\vec{r} g_v(\vec{r}) \hat{A}_v \left| \Phi^{(A-a,a)}_{vr} \right\rangle \]

Relative wave function (unknown)

Antisymmetrizer

\[ \psi^{(A-a)}_{\alpha_1} \psi^{(a)}_{\alpha_2} \delta(\vec{r} - \vec{r}_{A-a,a}) \]

Channel basis

Cluster expansion technique

Design to account for scattering states (best for long range correlations)

NCSMC
• Methods develop in this presentation to solve the many-body problem

\[ \Psi^{(A)}_{NCSM} = |A\lambda J^\pi T\rangle = \sum_{\alpha} c_\alpha |A\alpha j_z^\pi t_z\rangle \]

Mixing coefficients (unknown)

A-body harmonic oscillator states

\[ |A\lambda J^\pi T\rangle_{SD} \phi_{00}(\vec{R}_{c.m.}) \]

Second quantization

\[ \psi^{(A)}_{RGM} = \sum_v \int d\vec{r} g_v(\vec{r}) \hat{A}_v |\Phi^{(A-a,a)}_{v\vec{r}}\rangle \]

Relative wave function (unknown)

Antisymmetrizer

\[ \psi^{(A-a)}_{a_1} \psi^{(a)}_{a_2} \delta(\vec{r} - \vec{r}_{A-a,a}) \]

Channel basis

Cluster expansion technique

Adding three-cluster degrees of freedom:

\[ + \sum_v \int \int d\vec{x} d\vec{y} x^2 y^2 G_v(\vec{x}, \vec{y}) \hat{A}_v |\Phi^{(A-a_1-a_2,a_1,a_2)}_{v\vec{x}\vec{y}}\rangle \]

\[ \psi^{(A-a_1-a_2)}_{a_1} \psi^{(a_1)}_{a_2} \psi^{(a_2)}_{a_3} \delta(\vec{r} - \vec{r}_{a_1,a_2}) \times \delta(\vec{r} - \vec{r}_{A-a_12,a_12}) \]

Cluster expansion technique

\[ ^6\text{He properties: C. Romero-Redondo, et al. arXiv:1606.00066} \]
COUPLED NCSMC EQUATIONS

S. Baroni, P. Navrátil and S. Quaglioni PRL110 (2013); PRC93 (2013)

\[
\begin{pmatrix}
    H_{NCSM} & h \\
    h & H_{RGM}
\end{pmatrix}
\begin{pmatrix}
    \gamma
\end{pmatrix}
= E
\begin{pmatrix}
    1_{NCSM} & g \\
    g & N_{RGM}
\end{pmatrix}
\begin{pmatrix}
    \lambda \\
    \lambda'
\end{pmatrix}
\]

Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic R-matrix on Lagrange mesh
Translational invariance is preserved also with SD cluster basis

\[
SD \left\langle \Phi_f^{(A-a',a')} \right| \hat{O}_{t.i.} \left| \Phi_i^{(A-a,a)} \right\rangle_{SD} = \sum_{i_r f_r} M_{iSD fSD, i_r f_r} \left\langle \Phi_{f_r}^{(A-a',a')} \right| \hat{O}_{t.i.} \left| \Phi_{i_r}^{(A-a,a)} \right\rangle
\]

What we calculate in the “SD” channel basis

\[
\begin{pmatrix}
    \psi_{\alpha_1}^{(A-a)} \\
    \psi_{\alpha_2}^{(a)}
\end{pmatrix}_{SD} \varphi_{ni} \left( \vec{R}_{c.m.}^{(a)} \right)
\]

Observables calculated in the translationally invariant basis

\[
\begin{pmatrix}
    \psi_{\alpha_1}^{(A-a)} \\
    \psi_{\alpha_2}^{(a)}
\end{pmatrix} \varphi_{ni} \left( \vec{r}_{A-a,a} \right)
\]

- Advantage: can use powerful second quantization techniques

\[
SD \left\langle \Phi_{v'\eta'}^{(A-a',a')} \right| \hat{O}_{t.i.} \left| \Phi_{v\eta}^{(A-a,a)} \right\rangle_{SD} \propto SD \left\langle \Phi_{v'\eta'}^{(A-a',a')} \right| a_{A-a} a_{A-a} \left| \Phi_{v\eta}^{(A-a,a)} \right\rangle_{SD, SD} \left\langle \Phi_{v'\eta'}^{(A-a',a')} \right| a_{A-a} a_{A-a} \left| \Phi_{v\eta}^{(A-a,a)} \right\rangle_{SD} \ldots
\]
INCLUDING THE 3N FORCE INTO THE NCSM/RGM APPROACH
nucleon-nucleus formalism

\[
\langle \Phi^J_{v'r'} \mid \hat{A}' V^{NNN} \hat{A} \mid \Phi^J_{vr} \rangle = \begin{pmatrix} (A - 1) \\ (a' = 1) \end{pmatrix} \left| V^{NNN} \left( 1 - \sum_{i=1}^{A-1} \hat{P}_{iA} \right) \right| (a = 1) \]

\[
V^{NNN}_{\nu'\nu} (r, r') = \sum \mathcal{R}_{n'l'} (r') \mathcal{R}_{nl} (r) \left[ \frac{(A - 1)(A - 2)}{2} \right] \langle \Phi^J_{v'n'} | V_{A-2A-1A} (1 - 2P_{A-1A}) | \Phi^J_{vn} \rangle
\]

Direct potential:

\[
\propto_{SD} \langle \psi^{(A-1)}_{\alpha'_1} | a^\dagger a^\dagger aa | \psi^{(A-1)}_{\alpha_1} \rangle_{SD} \sim 1\text{Go}
\]

\[- \frac{(A - 1)(A - 2)(A - 3)}{2} \langle \Phi^J_{v'n'} | P_{A-1A} V_{A-3A-2A-1} | \Phi^J_{vn} \rangle \]

Exchange potential:

\[
\propto_{SD} \langle \psi^{(A-1)}_{\alpha'_1} | a^\dagger a^\dagger a^\dagger a \psi^{(A-1)}_{\alpha_1} \rangle_{SD} \sim \text{many two-body states}
\]
The 3N interactions influence mostly the $P$ waves.

The largest splitting between $P$ waves is obtained with NN+3N.

Comparison between NN+3N-ind and NN+3N at $N_{\text{max}}=13$ with six $^4$He states and 14 $^5$He states.
Study of the convergence with respect to the # of $^4$He low-lying states

- The convergence pattern looks good.
- The experimental phase-shifts are well reproduced.

$n^4$He scattering phase-shifts for NN+3N potential with $\lambda=2.0$ fm$^{-1}$ and first 14th low-lying state of $^5$He.
Experimental low-lying states of the $A=5$ nucleon systems.

- Convergence is rather slow.

Convergence of the phase shifts as a function of the $^4\text{He}$ excited states.
For the non-destructive physical, electrical and chemical characterization of materials, nuclear physics is routinely used for energies above the Rutherford scattering.

Impurities, e.g. $^4$He
Comparison of the $d$-$\alpha$ phase-shifts with different interactions ($N_{\text{max}}=11$)

- Best results in a decent model space ($N_{\text{max}}=11$).
- The $^3D_3$ resonance is reproduced but the $^3D_2$ and $^3D_1$ resonance positions are underestimated.
- The 3N force corrects the $D$-wave resonance positions by increasing the spin-orbit splitting.
- There is room for improvements.

$d^4\text{He}(g.s.)$ scattering phase-shifts for NN-only, NN+3N-induced, NN+3N-full potential with $\lambda=2.0$ fm$^{-1}$. 

$d^4\text{He}$ scattering
The 3N force is essential to get the correct $^6$Li g.s. energy and splitting between the $3^+$ and $2^+$ states.

The $^6$Li g.s. is well reproduced.

There is room for improvements, in particular regarding the $3^+$ state.
$^9$Be vs. $^9$Be+$^8$Be($0^+,2^+$) with chiral NN+3N(400) and $\lambda = 2.0$ fm$^{-1}$
$^9$Be vs. $^9$Be+$n$-$^8$Be(0$^+,2^+$) with chiral NN+3N(400) and $\lambda = 2.0$ fm$^{-1}$

THE COMBINATION OF THE TWO METHODS IS ESSENTIAL

J. Langhammer, P. Navrátil et al., PRC91 (2015)
In the shell model picture g.s. expected to be $J^{\pi}=1/2^{-}$ (Z=6, N=7) $^{13}$C and (Z=8, N=7) $^{15}$O have $J^{\pi}=1/2^{-}$ g.s.

In reality, $^{11}$Be g.s. is $J^{\pi}=1/2^{+}$ -- parity inversion

Very weakly bound: $E_{th}=-0.5$ MeV Halo state -- dominated by $^{10}$Be-n in the $S$-wave

The 1/2$^{-}$ state also bound -- only by 180 keV

Can we describe $^{11}$Be in *ab initio* calculations?

- Continuum must be included
- Does the 3N interaction play a role in the parity inversion?
$^{11}\text{Be}$ WITHIN NCSMC: DISCRIMINATION AMONG CHIRAL NUCLEAR FORCES

A. Calci, P. Navratil, G. Hupin, S. Quaglioni, R. Roth et al. with IRIS collaboration, in preparation

preliminary
n-^4^He phaseshifts with NCSMC and the chiral two- and three-nucleon force

- Perspective to provide accurate t(d,n)^4^He fusion cross-section for the effort toward earth-based fusion energy generation.
- The d-t fusion is known to be very sensitive to the spin-orbit and isospin part of the nuclear interaction.

n-^4^He(g.s.) phase shifts with NN+3N potential, \( \lambda=2.0 \) fm\(^{-1} \), with eigenstates of \(^5^He\) at \( N_{\text{max}} =9 \).
Towards d-t fusion with NCSMC: comparison between effective interactions

\[ \lambda = 1.7 \, \text{fm}^{-1} \text{ and } \hbar \Omega = 16 \, \text{MeV} \]

<table>
<thead>
<tr>
<th>N_{\text{max}}</th>
<th>^5\text{He} (\frac{3}{2}^+)</th>
<th>^4\text{He}</th>
<th>^3\text{H}</th>
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\[ \lambda = 2.0 \, \text{fm}^{-1} \text{ and } \hbar \Omega = 20 \, \text{MeV} \]

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<tr>
<th>N_{\text{max}}</th>
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</table>

NCSM convergence of compound and cluster states.

\( n^+^4\text{He}(\text{g.s.}) \) phase shifts with NN+3N potential, with eigenstates of \(^5\text{He}\).
Towards d-t fusion with NCSMC: comparison between effective interactions

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<tr>
<th>$N_{\text{max}}$</th>
<th>$^5\text{He (}^{3/2}_2\text{)}$</th>
<th>$^4\text{He}$</th>
<th>$^3\text{H}$</th>
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<td>-</td>
<td>0.02</td>
<td>2.06</td>
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$\lambda = 1.7 \text{ fm}^{-1}$ and $\hbar \Omega = 16 \text{ MeV}$

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$\lambda = 2.0 \text{ fm}^{-1}$ and $\hbar \Omega = 20 \text{ MeV}$

Relative error (%) with respect to converged value

A smaller frequency allows us to capture the dilute nature of the $^{3/2}_2^+$ resonance.

$n+^4\text{He(g.s.)}$ phase shifts with NN+3N potential, with eigenstates of $^5\text{He}$. 
Towards d-t fusion with NCSMC: comparison between effective interactions

The eigenvalue changes a huge amount but the eigenvector only changes a little.

C. Johnson, “Spectral distribution theory and the evolution of forces under the similarity renormalization group” at workshop “Progress in Ab Initio Techniques in Nuclear Physics” TRIUMF, Canada
**FIRST STEPS TOWARDS AB INITIO CALCULATIONS OF FUSION**

G. Hupin, S. Quaglioni, P. Navrátil work in progress

**Ab initio d-t fusion cross-section**

Preliminary..

Polarized cross-section will be a valued input to the design of energy based fusion technology.
FIRST STEPS TOWARDS AB INITIO CALCULATIONS OF FUSION
G. Hupin, S. Quaglioni, P. Navrátil work in progress

Ab initio d-t fusion cross-section

Cluster sector only
We are extending the *ab initio* NCSM/RGM approach to describe low-energy reactions with two- and three-nucleon interactions.

We are able to describe:

- Nucleon-nucleus collisions with NN+3N interaction
- Deuterium-nucleus collisions with NN+3N interaction as the n-n
- NCSMC for single- and two-nucleon projectile

**Work in progress:**

- Fusion reactions with our best complete *ab initio* approach
- The present NNN force is "incomplete", need to go to N³LO

Evolution of stars, birth, main sequence, death