Towards Unified Approaches to Nuclear Structure and Reactions for Nuclei

Guillaume Hupin

Collaborators
A. Calci (Industry)
J. Dohet-Eraly (Uni. Pisa)
J. Langhammer (Industry)
P. Navrátil (TRIUMF)
F. Raimondi (Uni. of Surrey)
C. Romero-Redondo (Industry)
R. Roth (TU Darmstadt)
S. Quaglioni (LLNL)
N. Pillet (CEA)
C. Robin (Uni. of Washington)
M. Dupuis (CEA)
V. Zelevinsky (MSU)

Ab initio
Exact
Configuration interaction
Nuclear energy density functional
MOTIVATIONS: DESCRIPTION OF EXOTIC (NEUTRON RICH) AND RESONANT SCATTERING

N. Michel, W. Nazarewicz, M. Płoszajczak et al. JPG36 (2008)
Methods developed in this presentation to solve the many-body problem:

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

- Mixing coefficients \((\text{unknown})\)
- A-body harmonic oscillator states
- Second quantization

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

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

Unable to describe observables sensitive to the tail of the w.f. and **continuum states**.
Methods developed in this presentation to solve the many body problem:

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

Mixing coefficients (unknown)

A-body harmonic oscillator states

Second quantization

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

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

Relative wave function (unknown)

Antisymmetrizer

Channel basis

Cluster expansion technique

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

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

NCSM/RGM

Cluster formalism for elastic/inelastic
UNDERSTANDING NUCLEAR STRUCTURE: $^6\text{Li}$
UNDERSTANDING NUCLEAR STRUCTURE: $^6\text{Li}$

No-Core Shell Model

Asymptotic conditions are exactly treated

$^4\text{He}+\text{d}$

3N force:

Extrapolation
• Consistent \textit{ab initio} calculation of this system.
• \textbf{Bound} and \textbf{resonant states} are treated in the same way.
• Effects of the chiral \textbf{3N force} are revealed.
Ability to probe the remaining inaccuracies of the nuclear interaction.

High accuracy is achieved in the low-energy limit, important for:

2. Radiative capture at low energy.
Possibility to discriminate between chiral nuclear forces?

Some of the shortcomings of the nuclear interaction can already be probed in $p$-shell nuclei through reactions. [NN $p$-waves are not perfectly reproduced by $N^2LO_{sat}$]

A. Kumar, R. Kanungo, A. Calci et al. PRL117 (2016).
The 3N interactions influence mostly the $P$ waves.

- The largest splitting between $P$ waves is obtained with $\text{NN+3N}$.

Comparison between $\text{NN+3N}$-ind and $\text{NN+3N}$ at $N_{\text{max}}=13$ with six $^4\text{He}$ states and 14 $^5\text{He}$ states.
Scattering phase shifts NCSM/FY

- Good agreement between the two methods.

Triangles from Faddeev-Yakubovsky
Courtesy of R. Lazauskas
- Bound states
- Resonant states
- Scattering states
- Halo densities
- Clusterizations
- ...
• Bound states
• Resonant states
• Scattering states
• Halo densities
• Clusterizations
• ...

Carolina Romero-Redondo et al. PRL113 (2014); PRL117 (2016)
La science doit « nous rendre comme maîtres et possesseurs de la Nature »
R. Descartes *Discours de la méthode.*

ITER design (Cadarache, France)
The importance of the structure of neighboring resonances is revealed in transfer reactions. The structure of the $^5\text{He} \ ^3/2^+$ resonance is shown, with excitation to $0\,^p^1\!\!0\,^p^3\!\!0\,^{1h}$. There is no $^5\text{He}$ structure. S-factor and angular distribution are depicted for a range of energies.
Reactant spins are prepared in a given configuration.

\[
\sigma_{\text{polar}}(\theta) = \sigma(\theta) \left( 1 + \frac{1}{3} p_{zz} A_{zz} + \frac{3}{2} p_z p_{zt} C_{z,z^t} \right)
\]

- **Importance** of structure of neighboring resonances is revealed in transfer reactions.
- **Predictions** for \(^3\text{He}(d,n)^4\text{He}\) reaction and its enhancement factor.

G. Hupin, S. Quaglioni and P. Navrátil to be submitted
Angular distribution in different polarization scenarios

Spin tensor properties of the deuteron give the angular shape.
(Same as in $^3\text{He}(\vec{d},p)^4\text{He}$)

- $J = 1/2$  
  $J_z = -1/2$

- $J = 1$  
  $J_z = 1$

Total cross section increased
(on average) No changes
Total cross section decreased
\[ \Psi^{(A)}_{(F)CI} = |A\lambda J^\pi T\rangle = \sum_\alpha c_\alpha |A\alpha j_z^\pi t_z\rangle \]

Mixing coefficients (unknown)

A-body harmonic oscillator states

Second quantization

The MPMH is a double variational method

Variational amplitudes are the mixing coef. \( c_\alpha \) and the single-particle orbitals \( \phi_i(r_i) \), i.e.

\[ \frac{\partial E}{\partial c_\alpha} = \frac{\partial E}{\partial \phi_i} = 0 \]

\[ \Psi^{(A)}_{MPMH} = \sum_\alpha c_\alpha A_\alpha \phi_{\alpha,A}(r_A)\phi_{\alpha,A-1}(r_{A-1}) \ldots \phi_{\alpha,1}(r_1) \]

Mixing coefficients (unknown)

Single particle states (unknown)
For computational purpose we can truncate further

- Based on many-body energy:

\[
\Psi^{(A)}_{MPMH} = \sum_{\alpha} c_{\alpha} A_{\alpha} \varphi_{\alpha,A}(\vec{r}_A) \varphi_{\alpha,A-1}(\vec{r}_{A-1}) \ldots \varphi_{\alpha,1}(\vec{r}_1)
\]

- Maximum s.p. energy

\[
\Psi^{(A)}_{MPMH} = \sum_{\alpha=\alpha_{\text{max}}}^{\alpha_{\text{max}}} c_{\alpha} A_{\alpha} \varphi_{\alpha,A}(\vec{r}_A) \varphi_{\alpha,A-1}(\vec{r}_{A-1}) \ldots \varphi_{\alpha,1}(\vec{r}_1)
\]
For computational purpose we can truncate further

- Based on many-body energy:

$$\Psi^{(A)}_{MPMH} = \sum_{\alpha} c_{\alpha} A_{\alpha} \varphi_{\alpha,A}(\vec{r}_{A}) \varphi_{\alpha,A-1}(\vec{r}_{A-1}) \ldots \varphi_{\alpha,1}(\vec{r}_{1})$$

- Based on an active valence space and inactive core:

$$\Psi^{(A)}_{MPMH} = \sum_{\alpha=\alpha_{\text{min}}}^{\alpha_{\text{max}}} c_{\alpha} \Phi_{\alpha,N}(\vec{r}_{A-a}, \ldots, \vec{r}_{A}) \Phi_{A-N}(\vec{r}_{1}, \ldots, \vec{r}_{A-a})$$

**MPMH METHOD: BRIEF INTRO**
MPMH METHOD: BRIEF INTRO

✓ According to the type of many-body excitations

- All nuclear correlations thought to be important in mean-field can be included.

- Some key features:
  - Systematically improvable, i.e. all the Hilbert space can be spanned.
  - All symmetries but translational invariance are conserved.
**Variation of mixing coefficients:** large-scale diagonalization.

\[ \delta c^*_\alpha \left( E[\Psi] - \lambda(\langle\Psi|\Psi\rangle - 1) \right) = 0 \]

\[ \Leftrightarrow \sum_{\beta} \langle \Phi_\alpha | H | \Phi_\beta \rangle c_\beta = \lambda c_\alpha \]

**Variation of orbitals:**

generalized one-body problem embedded in many-body space spanned by \( \Psi \).

\[ \delta \varphi^*_i \left( E[\Psi] - \lambda(\langle\Psi|\Psi\rangle - 1) \right) = 0 \]

\[ \Leftrightarrow [h[\rho], \rho] = G[\sigma] \]

Orbitals are optimum: \( |\varphi\rangle = U|\varphi\rangle \)

**Mean-field** adapted to a given type of many-body correlations (NCSMC, Shell-Model, 2p-2h...).

Opt. orbital

HO states

Illustration

Ch. Constantinou, M. A. Caprio et al. arXiv:1605.04976
use MPMH for the first time:
- To renormalize a bare nuclear interaction and **reveal** the corresponding **mean-field**.
- MPMH can treat beyond mean-field correlations.
**Ab initio → Mean field**

use MPMH for the first time:
- To renormalize a bare nuclear interaction and **reveal** the corresponding mean-field.

→ MPMH can treat beyond mean-field correlations.
→ Need for a more general functional form (yet easy to integrate).

\[ v_{12}[\rho] = \sum_{j=1}^{2} \left( W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau \right) e^{-\frac{(|\vec{r}_1 - \vec{r}_2)|^2}{\mu_j}} \]

\[ + \left( W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau \right) e^{-\frac{(|\vec{r}_1 - \vec{r}_2)|^2}{\mu_3}} \frac{\rho^\alpha (r_1) + \rho^\alpha (r_2)}{2(\mu_3 \pi)^{3/2}} \]

\[ + iW_{LS} \vec{v}_{12} \delta (\vec{r}_1 - \vec{r}_2) \wedge \vec{v}_{12} (\vec{\sigma}_1 + \vec{\sigma}_2) \]

+ tensor

**CONNECTING EDF TO BARE INTERACTION WITH MPMH**

Courtesy of N. Pillet
Use MPMH for the first time:

- To renormalize a bare nuclear interaction and reveal the corresponding mean-field.
- MPMH can treat beyond mean-field correlations.
- Need for a more general functional form (yet easy to integrate).

$$v_{12}[\rho] = \sum_{j=1}^{2} \left( W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau \right) e^{-(\vec{r}_1 - \vec{r}_2)^2/\mu_j}$$

$$+ (W_j + B_j P_\sigma - H_j P_\tau - M_j P_\sigma P_\tau) e^{-(\vec{r}_1 - \vec{r}_2)^2/\mu_3} \frac{\rho^\alpha(r_1) + \rho^\alpha(r_2)}{2(\mu_3 \pi)^{3/2}}$$

$$+ iW_{LS} \vec{v}_{12} \delta(\vec{r}_1 - \vec{r}_2) \wedge \vec{v}_{12} (\vec{\sigma}_1 + \vec{\sigma}_2)$$

- Use properties of the continuum to infer an interaction fitted for exotic systems: a first step towards reactions.

**Ab initio ➔ Mean field**

**Continuum properties of $^{11}$N**

<table>
<thead>
<tr>
<th>$J^\pi$</th>
<th>$E_r$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\Gamma$</th>
<th>$E_r$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2$^+$</td>
<td>1.47</td>
<td>5.53</td>
<td>1.33</td>
<td>1.45</td>
<td>1.49(6)</td>
<td>0.83(3)</td>
</tr>
<tr>
<td>1/2$^-$</td>
<td>1.91</td>
<td>0.55</td>
<td>1.95</td>
<td>0.57</td>
<td>2.22(3)</td>
<td>0.6(1)</td>
</tr>
</tbody>
</table>

*Courtesy of N. Pillet*
The complex scaling and the resonance states

\[ \hat{H}(r) = \hat{T} + \hat{V}(r) \]

\[ \hat{H}(\theta) = e^{-2i\theta \hat{T}} + \hat{V}(re^{i\theta}) \]
\[ \hat{H}(r) = \hat{U}(\theta)\hat{H}(r)\hat{U}^{-1}(\theta) \]

**Aguilar-Balslev-Combes theorem:** the resonant states of the original Hamiltonian are invariant and the non-resonant scattering states are rotated and distributed on a 2\( \theta \) ray that cuts the complex energy plane with a corresponding threshold being the rotation point.

\[ \hat{H}(r, \theta)\psi(r, \theta) = (E + i\Gamma)\psi(r, \theta) \]

Energy \( \uparrow \) Half-life
The complex scaling and the resonance states

\[ \hat{H}(r) = \hat{T} + \hat{V}(r) \]

\[ \hat{H}(\theta) = e^{-2i\theta} \hat{T} + \hat{V}(re^{i\theta}) \]

\[ \hat{H}(r) = \hat{U}(\theta) \hat{H}(r) \hat{U}(\theta)^{-1} \]

\[ \psi(r, \theta) \sim e^{-kr \sin \theta} \]

Spatially extended but falls off exponentially

Boundary limit problem

Bound state problem
Schematic case: the deuteron
- Use of an HO basis in Jacobi coordinates
- Diagonalization in the deuteron channel

Generalization of the MPMH configuration mixing approach to symmetric non-hermitian complex matrices.

Collaboration with R. Lazauskas and J. Carbonell
• SRG evolution requires spanning a large NN basis ($n_r \sim 150$). The typical scale of $k$ is 10 fm$^{-1}$ ($V^{NN}$).

• Complex scaling involves the integration of diverging polynomials (of order $n$) far from their zeroes.
SOFT INTERACTION FOR CI METHODS WITH SRG

$^1S_0$ N$^3$LO pn interaction at $\theta = 10.0^\circ$, $\Lambda_{\text{SRG}} = 1.5 \text{ fm}^{-1}$
With core polarization effects