Ab initio calculations of reactions and exotic nuclei

Toward Predictive Theories of Nuclear Reactions Across the Isotopic Chart (INT 17-1a)

Sofia Quaglioni
A predictive theory of light-nuclei reactions is essential for both basic and applied science

What is the nature of the nuclear force?

Standard solar model

Fusion Technology

Life's building blocks

Carbon and Oxygen

Helium Burning Shell

\[ \alpha + \alpha + \alpha \rightarrow ^{12}\text{C} + \gamma \]

\[ \alpha + ^{12}\text{C} \rightarrow ^{16}\text{O} + \gamma \]

\[ ^{3}\text{H} + ^{3}\text{H} \rightarrow ^{4}\text{He} + 2n \]

\[ d + ^{3}\text{H} \rightarrow ^{4}\text{He} + n \]

\[ ^{3}\text{He} + ^{4}\text{He} \rightarrow ^{7}\text{Be} + \gamma \]

\[ ^{7}\text{Be} + p \rightarrow ^{8}\text{B} + \gamma \]

\[ ^{7}\text{Be} + e^{-} \rightarrow ^{7}\text{Li} + \nu_e \]

\[ ^{7}\text{Li} + p \rightarrow ^{4}\text{He} + ^{4}\text{He} \]

\[ ^{3}\text{He} + ^{4}\text{He} \rightarrow ^{7}\text{Be} + \gamma \]

\[ ^{8}\text{B} \rightarrow ^{8}\text{Be} + e^{-} + \nu_e \]

\[ ^{8}\text{Be}^* \rightarrow ^{4}\text{He} + ^{4}\text{He} \]
Our problem: quantum mechanical scattering. The ‘idealist’ and the ‘pragmatic’ approach

Ab Initio Theory

- A nucleon degrees of freedom
- ‘Realistic’ nucleon-nucleon (NN) and three-nucleon (3N) forces
- Pauli principle treated exactly
- Extremely difficult multichannel scattering problem
  - Exactly solvable for $A = 3,4$
  - What to do for heavier light nuclei?

Few-Body Model

- Few (3 or 4) relevant ‘cluster’ d.o.f.
- Structure of clusters is neglected
- Effective (optical) potential between core, valence and target
- Pauli principle approximated
- Easier to solve, more widely applicable
1) Reconstruct the interaction potential between a projectile and a target starting from:
   - *Ab initio* square-integrable wave functions of the clusters
   - ‘Realistic’ nucleon-nucleon (NN) and three-nucleon (3N) interactions

2) Solve for projectile-target relative motion

At low-energies, when only a few reaction channels are open, ‘adiabatic’ two-step solution

Energy

\[ E > 0 \]
\[ E_2 < 0 \]
\[ E_1 < 0 \]

Overall interaction potential between projectile and target

This is the main concept behind the no-core shell model with continuum approach ... albeit with a small tweak
Ab initio no-core shell model with continuum (NCSMC)

- Seeks many-body solutions in the form of a generalized cluster expansion

\[ \Psi^{(A)} = \sum_{\lambda} c_{\lambda} |A,\lambda \rangle + \sum_{\nu} \int d\vec{r} \ u_{\nu}(\vec{r}) \hat{A}_{\nu} |A-a,\nu \rangle \]

- **Ab initio** no-core shell model (NCSM):
  - Clusters’ structure, short range

- Resonating-group method (RGM):
  - Dynamics between clusters, long range
Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations

- Scattering matrix (and observables) from matching solutions to known asymptotic with microscopic $R$-matrix on Lagrange mesh
Discrete and continuous variational amplitudes are determined by solving the coupled NCSMC equations

\[ H_{\text{NCSM}} h = E \begin{pmatrix} 1_{\text{NCSM}} \\ g \end{pmatrix} \]
A few words about the RGM portion of the basis

- NCSMC generalized cluster expansion:

\[ \Psi^{(A)} = \sum_{\lambda} c_{\lambda} (A)_{\lambda} + \sum_{\nu} \int d\vec{r} u_{\nu}(\vec{r}) \hat{A}_{\nu} (A-a)_{\nu} \]

Ununknowns

- These are translational invariant basis states, describing only the internal motion

- Note: Here the target and projectile are both translational invariant states
Since we are using NCSM eigenstates, it is convenient to introduce HO channel states

- Jacobi channel states in the harmonic oscillator (HO) space:

\[ \Phi_{vn}^{J^T} = \left[ \left( | A - a \alpha_1 I_1^{\pi_1} T_1 \rangle \langle a \alpha_2 I_2^{\pi_2} T_2 \right) \left| Y_\ell \left( \hat{r}_{A-a,a} \right) \right| R_{n\ell} \left( r_{A-a,a} \right) \right]^{(J^T)} \]

- Notes:

  - Formally, the coordinate space channel states given by:

\[ \Phi_{vr}^{J^T} = \sum_n \left| R_{n\ell} \right( r \right) \Phi_{vn}^{J^T} \]

    - I used the closure properties of HO radial wave functions

\[ \delta(r - r_{A-a,a}) = \sum_n R_{n\ell}(r) R_{n\ell}(r_{A-a,a}) \]

  - Again: target and projectile are both translational invariant eigenstates

    - Works for the projectiles up to $^4\text{He}$

    - Not practical if we want to describe reactions with p-shell targets!

In practice, expansion is truncated and only works for short-range components of NCSM/RGM kernels.
An example: the RGM norm kernel for nucleon-nucleus channel states

\[
\langle \Phi_{\nu'\nu}^{J^{\pi}_T} | \hat{A}_{\nu'} \hat{A}_{\nu} | \Phi_{\nu\nu}^{J^{\pi}_T} \rangle = \left\langle \begin{array}{c} (A-1) \\ r' (a' = 1) \end{array} \right| 1 - \sum_{i=1}^{A-1} \hat{P}_{ia} | (a = 1) \rangle \left\langle \begin{array}{c} (A-1) \\ r \end{array} \right|
\]

\[
N_{v'v}^{\text{RGM}} (r', r) = \delta_{v'v} \frac{\delta (r' - r)}{r'r} - (A-1) \sum_{n'n} R_{n'\ell} (r') R_{n\ell} (r) \langle \Phi_{v'n'}^{J^{\pi}_T} | \hat{P}_{A-1,A} | \Phi_{vn}^{J^{\pi}_T} \rangle
\]

**Direct term:** Treated exactly! (in the full space)

**Exchange term:** Obtained in the model space! 
(Short-range many-body correction due to the exchange of particles)

\[
\delta (r - r_{A-a,a}) = \sum_{n} R_{n\ell} (r) R_{n\ell} (r_{A-a,a})
\]
Define Slater-Determinant (SD) channel states in which the target is described by a SD eigenstates

$$\left| \Phi_{vn}^{J\pi_T} \right\rangle_{SD} = \left( \left| A - a \alpha_1 I_1^{\pi_1} T_1 \right\rangle_{SD} | a \alpha_2 I_2^{\pi_2} T_2 \right\rangle \right)^{(sT)} Y_{\ell} \left( \hat{R}^{(a)}_{c.m.} \right) \left| R_n \right\rangle \left( R^{(a)}_{c.m.} \right)$$

Vector proportional to the c.m. coordinate of the $A-a$ nucleons

$$\left| A - a \alpha_1 I_1^{\pi_1} T_1 \right\rangle \varphi_{00} \left( \hat{R}^{(A-a)}_{c.m.} \right)$$

Vector proportional to the c.m. coordinate of the $a$ nucleons

$$(A-a) \quad \xi_0 \Rightarrow \hat{R}^{(A)}_{c.m.} \equiv \frac{n}{A-a} \quad (a)$$

$$\left( \varphi_{00} \left( \hat{R}^{(A-a)}_{c.m.} \right) \varphi_{n\ell} \left( \hat{R}^{(a)}_{c.m.} \right) \right)^{\ell} = \sum_{n_r \ell_r, NL} \left\langle 00, n \ell, \ell \left| n_r, \ell_r, NL, \ell \right\rangle \right\rangle_{d=A-a} \left( \varphi_{n_r \ell_r} \left( \hat{\eta}_{A-a} \right) \varphi_{NL} \left( \xi_0 \right) \right)^{\ell}$$

motion
In this ‘SD’ channel basis, translation-invariant matrix elements are mixed with c.m. motion ...

- More in detail:

\[
\Phi_{vn}^{\pi T} \rangle_{SD} = \sum_{n_r, \ell_r, NL, J_r} \hat{\ell} \hat{J}_r (-1)^{s+\ell_r+L+J} \begin{pmatrix} s & \ell_r & J_r \\ L & J & \ell \end{pmatrix} \langle 00, n_\ell, \ell | n_{\ell_r}, NL, \ell \rangle_{d_{a-A}} [ \Phi_{v_r n_r}^{\pi T} \varphi_{NL}(\vec{\xi}_0) ]^{(\pi T)}
\]

- The spurious motion of the c.m. is mixed with the intrinsic motion

\[
\sum_{n_r', \ell_r', n_{\ell_r'}, J_{\ell_r'}} \langle \Phi_{v_r' n_r'}^{\pi T} | \hat{O}_{t,i} | \Phi_{v_n n_r}^{\pi T} \rangle_{SD} = \sum_{n_r', \ell_r', n_{\ell_r'}, J_{\ell_r'}} \langle \Phi_{v_r' n_r'}^{\pi T} | \hat{O}_{t,i} | \Phi_{v_r' n_r}^{\pi T} \rangle_{SD}
\]

Interested in this

Compute these

\[
\times \sum_{NL} \hat{\ell} \hat{\ell'} \hat{J}_r^2 (-1)^{s+\ell'-s'-\ell'} \begin{pmatrix} s & \ell_r & J_r \\ L & J & \ell' \end{pmatrix} \begin{pmatrix} s' & \ell'_r & J_r \\ L & J & \ell' \end{pmatrix} \times \langle 00, n_\ell, \ell | n_{\ell_r}, NL, \ell \rangle_{d_{a-A}} \langle 00, n'_{\ell'}, \ell' | n'_{\ell_r'}, NL, \ell' \rangle_{d'_{a-A}}
\]
... but they can be extracted exactly from the ‘SD’ matrix elements by applying the inverse of the mixing matrix

- More in detail:

\[
\begin{align*}
\left| \Phi_{vn}^{J\pi T} \right\rangle_{SD} &= \sum_{n_r, \ell_r, NLJ_r} \hat{\ell}\hat{J}_r (-1)^{s+\ell_r+L+J} \begin{pmatrix} S & \ell_r & J_r \\ L & J & \ell \end{pmatrix} \langle 00, n\ell, \ell | n_r \ell_r, NL, \ell \rangle_{d=\frac{a_A}{a}} \left[ \Phi_{v_r n_r}^{J_{\pi T}} \phi_{NL} (\tilde{\xi}_0) \right]^{(J_{\pi T})}
\end{align*}
\]

- The spurious motion of the c.m. is mixed with the intrinsic motion

Matrix inversion

\[
\begin{align*}
\langle SD | \hat{O}_{t.i.} | \Phi_{f SD}^{J\pi T} \rangle &= \sum_{i_R f_R} M_{i_SD f_SD}^{J_{\pi T}} \langle SD | \hat{O}_{t.i.} | \Phi_{i_R}^{J_{\pi T}} \rangle
\end{align*}
\]

Calculate these

Interested in these
Working within the ‘SD’ channel basis we can access reactions involving p-shell targets

- Can use second quantization representation

  - Matrix elements of translational operators can be expressed in terms of matrix elements of density operators on the target eigenstates

  - E.g., the matrix elements appearing in the RGM norm kernel for nucleon-nucleus channel states:

  \[
  SD \left< \Phi^{J^T}_{\nu n'} \middle| P_{A-1,A} \middle| \Phi^{J^T}_{\nu n} \right>_{SD} = \frac{1}{A-1} \sum_{j'jK\tau} \hat{s}\hat{s}'\hat{j}\hat{j}'\hat{\kappa}\hat{\tau} (-1)^{l'+j'+J} (-1)^{T_{1}+\frac{1}{2}+T} \times \left< A-1 \alpha_{i} I_{1}^{T'} T_{1} \middle| \left( a_{n\ell j_{1}}^{+} \tilde{a}_{n'\ell' j_{1}'} \right)^{(K\tau)} \middle| A-1 \alpha_{i} I_{1}^{T} T_{1} \right>_{SD}
  \]

  One-body density matrix elements
In the following I will review some results

Adopted interactions:

- **NN**: potential at $N^3$LO, 500 MeV cutoff (by Entem & Machleidt)

- **NN+3N(500)**: NN plus 3N force at $N^2$LO, 500 MeV cutoff (local form by Navrátil)

- **NN+3N(400)**: NN plus 3N force at $N^2$LO, 400 MeV cutoff (local form by Navrátil)

- **$N^2$LOsat**: NN+3N at $N^2$LO, fitted simultaneously (by Ekström et al.)

Chiral Effective Field Theory

Worked out by Van Kolck, Keiser, Meissner, Epelbaum, Machleidt, ...
Neutron-$^4$He scattering: a magnifying glass for 3N forces

- 3N force enhances $1/2^- \leftrightarrow 3/2^-$ splitting; essential at low energies!

Elastic scattering of neutrons on $^4$He

Neutron-$^4\text{He}$ scattering: a magnifying glass for 3N forces

- $1/2^- \leftrightarrow 3/2^-$ splitting sensitive to 3N force, strength of spin-orbit

Elastic scattering of neutrons on $^4\text{He}$

We can reproduce the elastic scattering and recoil of protons off $^4$He based on chiral NN+3N(500) interactions

- Used to characterize $^1$H and $^4$He impurities in materials’ surfaces

Elastic scattering and recoil of deuterons off $^4\text{He}$

- Narrow $3^+$ resonance not well described by NN+3N(500) force

Opportunity to root three-body reaction model in ab initio many-body framework (F. Nunes)

Ab initio many-body → Three-Body Model

- 3 relevant ‘cluster’ d.o.f.
- Structure of target is neglected
- Effective (optical) potential between nucleons and target
- Pauli principle approximated
- Expect need for effective 3-body force to recover ab initio results

Elastic d-^4^He Scattering

<table>
<thead>
<tr>
<th>Energy (MeV)</th>
<th>Plot</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.93</td>
<td><img src="c" alt="Plot" /></td>
</tr>
<tr>
<td>6.96</td>
<td><img src="c" alt="Plot" /></td>
</tr>
<tr>
<td>8.97</td>
<td><img src="c" alt="Plot" /></td>
</tr>
<tr>
<td>12.0</td>
<td><img src="c" alt="Plot" /></td>
</tr>
</tbody>
</table>

\(4^He(d,d)^4^He\)

\([\sigma/\Omega]_{c.m.}\) in [b/sr]

\(\theta_d\) [deg]

\(NN+3N(500)\)
What is more important in shaping energy spectra: the proximity to a breakup threshold or 3N-force effects?

- The $^6$Li ground state lies only 1.47 MeV (compared to its absolute binding energy of nearly 32 MeV) below the $^4$He+d separation energy.

- To find answer, we compared energies obtained with and without the coupling of d+$^4$He continuum states.

It would be interesting to compare with symmetry-adapted NCSM.

$^6\text{Li}$ asymptotic $D$- to $S$-state ratio in $d^4\text{He}$ configuration

- In the NCSMC, bound state wave functions have (correct) Whittaker asymptotic -- as opposed to traditional NCSM!

$$u_c(r) = C_c W(k_c r)$$

- Asymptotic $D$- to $S$-state ratio ($C_2/C_0$) of $^6\text{Li}$ g.s. in $d^4\text{He}$ configuration
  - Not well determined, even as to its sign
  - Our results do not support a near-zero value

<table>
<thead>
<tr>
<th>$^6\text{Li}(\text{g.s.})$</th>
<th>NCSMC</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$ [MeV]</td>
<td>-32.01</td>
<td>-31.994</td>
</tr>
<tr>
<td>$C_0$ [fm$^{-1/2}$]</td>
<td>2.695</td>
<td>2.91(9)</td>
</tr>
<tr>
<td>$C_2$ [fm$^{-1/2}$]</td>
<td>-0.074</td>
<td>-0.077(18)</td>
</tr>
<tr>
<td>$C_2/C_0$</td>
<td>-0.027</td>
<td>-0.025(6)(10)</td>
</tr>
</tbody>
</table>


George & Knutson, PRC 59, 598 (1999): Determination from $^6\text{Li}d$ elastic scattering

K.D. Veal et al., PRL 81, 1187 (1998): Determination from $(^6\text{Li},d)$ reactions on medium-heavy targets.
With the same NN+3N forces, we can also make predictions for more complex transfer reactions

- Deuterium-Tritium fusion
  - Big Bang nucleosynthesis of light nuclei
  - Fusion research and plasma physics

- What is the effect of spin polarization on the reaction rate?

\[
N_A \langle \sigma v \rangle = \frac{8}{\pi \mu} \left( \frac{N_A}{k_B T} \right)^{3/2} \int_0^\infty dE \ S(E) \ \exp \left( -\frac{2\pi Z_1 Z_2 e^2}{\hbar \sqrt{2mE}} - \frac{E}{k_B T} \right)
\]

G. Hupin, S. Quaglioni, and P. Navrátil, in progress
Can ab initio theory explain the phenomenon of parity inversion in $^{11}\text{Be}$?

Phenomenologically adjusted NCSMC

NCSM energy eigenvalues treated as adjustable parameters; clusters’ excitation energies set to experimental value
Can ab initio theory explain the photodisintegration of $^{11}$Be?

Opportunity to arrive at a more realistic description of the projectile in few-body models

**Few-Body Model**

- Few (3 or 4) relevant ‘cluster’ d.o.f.
- Structure of clusters is neglected
- Effective (optical) potential between core, valence and target
- Pauli principle approximated
- Easier to solve, more widely applicable

**Semi-microscopic model**

- Structure of target is still neglected
- Connection to ab initio many-body theory for the projectile
- Ab initio wave functions (S-matrix) of projectile (see talk of A. Bonaccorso)
- Effective valence-core interaction fitted to ab initio phase shifts (see talk of P. Capel)
Now gradually building up capability to describe solar pp-chain reactions

The $^3\text{He}(\alpha,\gamma)^7\text{Be}$ fusion rate is essential to evaluate the fraction of pp-chain terminations resulting in $^7\text{Be}$ versus $^8\text{B}$ solar neutrinos

- Quantitative comparison still requires inclusion of 3N forces

**Ab initio** calculations simultaneously address many-body correlations and 3-cluster dynamics

**Borromean halos (dripline nuclei)**

- $^6\text{He} (= ^4\text{He}+n+n)$,
- $^{11}\text{Li} (= ^9\text{Li}+n+n)$,
- $^{14}\text{Be} (= ^{12}\text{Be}+n+n)$,
- ...  
- Constituents do not bind in pairs!

- 3-cluster NCSMC

---

**Ab initio** calculations simultaneously address many-body correlations and 3-cluster dynamics

**Borromean halos** *(dripline nuclei)*

- $^6\text{He} (= ^4\text{He}+n+n)$,  
  $^{11}\text{Li} (= ^9\text{Li}+n+n)$,  
  $^{14}\text{Be} (= ^{12}\text{Be}+n+n)$,  
  ...

- Constituents do not bind in pairs!

- 3-cluster NCSMC

---

Ab initio calculations simultaneously address many-body correlations and 3-cluster dynamics.

Quantitative comparison still requires inclusion of 3N forces.
Conclusions and Prospects

- Working within the ab initio no-core shell model with continuum we have made great strides in the description of reactions and exotic nuclei
- We are on the verge of predicting Solar fusion cross sections and reaction rates for fusion technology from chiral NN+3N forces
- These developments are also allowing to further expose and will help overcome deficiencies in chiral NN+3N forces
- New opportunities to forge a connection between ab initio many-body theory and few-body reaction models are emerging
Collaborators

- A. Calci (TRIUMF)
- J. Dohet-Eraly (INFN Pisa)
- G. Hupin (CEA, DAM, DIF)
- W. Horiuchi (Hokkaido U)
- P. Navratil (TRIUMF)
- C. Romero-Redondo (LLNL)
- R. Roth (TU Darmstadt)