Advances on NCSM, SRG & Chiral Interactions

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Ab Initio Workflow

Nuclear Structure & Reaction Observables

- Many-Body Solution via NCSM, CC, IM-SRG,...
  - initial formulation typically limited to bound-state basis
  - description of continuum effects and observables not possible
  - improvement: include continuum degrees of freedom explicitly
  - here: NCSM with Continuum

Similarity Renormalization Group

NN+3N Interactions from Chiral EFT

Low-Energy QCD
Ab Initio Workflow

**Nuclear Structure & Reaction Observables**

- Many-Body Solution via NCSM, CC, IM-SRG, ...
- Similarity Renormalization Group
- NN+3N Interactions from Chiral EFT

**Low-Energy QCD**

- Drastically improves convergence but induces many-body forces
- Induced beyond-3N interactions are a major limitation for many applications
- Improvement: either include or suppress induced forces
- Here: **Block Generators**
Ab Initio Workflow

**Nuclear Structure & Reaction Observables**

- Many-Body Solution via NCSM, CC, IM-SRG, ...
- Similarity Renormalization Group
- NN+3N Interactions from Chiral EFT

**Low-Energy QCD**

- chiral EFT offers systematics, improvability and uncertainty estimation
- typically one "chiral interaction" is used in nuclear structure
- improved chiral EFT interactions offer opportunity to quantify uncertainties systematically
- here: initial NCSM studies with NN from LO to N4LO
NCSM with Continuum for the Structure of $^9$Be

with
J. Langhammer, P. Navrátil,
S. Quaglioni, G. Hupin, A. Calci

NCSM with Continuum

comprehensive ab initio description of light nuclei

bound states & spectroscopy

(IT-)NCSM
ab initio description of nuclear clusters

resonances & scattering states

RGM
describing relative motion of clusters

focus on NCSMC with 3N interactions for p-shell spectroscopy

NCSMC with 3N Forces

representing $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **over-complete basis**

$$|\psi^{J\pi T}\rangle = \sum_{\lambda} c_{\lambda} |\Psi_A E_\lambda J^{\pi T}\rangle + \sum_{\nu} \int dr r^2 \frac{\chi_r(r)}{r} |\xi^{J\pi T}_{\nu r}\rangle$$

leads to the **NCSMC equations**

$$\begin{pmatrix} H_{\text{NCSM}} & h \\ h & \mathcal{H} \end{pmatrix} \begin{pmatrix} c \\ \chi(r)/r \end{pmatrix} = 0$$

with 3N contributions in

- $H_{\text{NCSM}}$
- $h$
- $\mathcal{H}$

covered by (IT-)NCSM

given by $\langle \Psi_A E_\lambda J^{\pi T} | \hat{H} |\xi^{J\pi T}_{\nu r}\rangle$

contains NCSM/RGM Hamiltonian kernel

access targets beyond $^4$He using uncoupled densities and on-the-fly algorithm.
Ab Initio Description of $^9$Be

- $^9$Be is excellent candidate to study continuum effects on spectra
- all excited states are resonances
- previous NCSM studies with NN interactions show clear discrepancies in spectrum: 3N or continuum effects?
- include n-$^8$Be continuum in NCSMC
- use standard NN+3N Hamiltonian:
  - NN: N3LO, Entem & Machleidt, 500 MeV cutoff
  - 3N: N2LO, Local, 500 MeV cutoff
**9Be: Convergence of Phase Shifts**

- include $0^+$, $2^+$ states of $^8$Be
- include 6 negative and 4 positive parity states of $^9$Be
- negative parity phase-shifts are well converged, positive parity more difficult
- extract resonance parameters from inflection point and derivative

\[ \alpha = 0.0625 \text{ fm}^4, \quad \hbar \Omega = 20 \text{ MeV}, \quad E_{3\text{max}} = 14 \]
9Be: NCSM vs. NCSMC

- NCSMC shows much better $N_{\text{max}}$ convergence
- NCSM tries to capture continuum effects via large $N_{\text{max}}$
- drastic difference for the $1/2^+$ state right at threshold

Langhammer, Navrátil, Quaglioni, Hupin, Calci, Roth; Phys. Rev. C 91, 021301(R) (2015)
continuum plays more important role than chiral 3N interaction

NCSMC predictions for widths are in fair agreement with experiment
SRG with Block Generators

with
A. Calci, N. M. Dicaire, C. Omand, P. Navrátil,
T. Hüther, S. Schulz, K. Vobig
continuous unitary transformation to pre-diagonalize Hamiltonian and thus improve model-space convergence

- **consistent unitary transformation** of Hamiltonian and observables
  \[ H_\alpha = U_\alpha^\dagger H U_\alpha \quad \text{and} \quad O_\alpha = U_\alpha^\dagger O U_\alpha \]

- evolution equations for \( H_\alpha \) and \( U_\alpha \)
  \[ \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \quad \frac{d}{d\alpha} O_\alpha = [\eta_\alpha, O_\alpha] \]

- **dynamic generator** \( \eta_\alpha \) drives towards “diagonal” defined by \( G_\alpha \)
  \[ \eta_\alpha = (2\mu)^2 [G_\alpha, H_\alpha] \]

- design \( G_\alpha \) for optimum compromise between convergence & induced many-body forces
Choice of Generator: $T_{\text{int}}$

- standard choice for $G_\alpha$ is **intrinsic kinetic energy** $T_{\text{int}}$
- drives diagonalization everywhere, also for low-lying basis states that are covered explicitly by many-body model space
- rule of thumb: the more diagonal the more induced many-body interactions

*HO matrix elements, $^1S_0$ channel, $\hbar \Omega = 24$ MeV*
Choice of Generator: Block Generators

**HO block generator**: use $H_\alpha$ matrix elements for states below $N_{gen}$ and $T_{int}$ matrix elements above, i.e.,

$$G_\alpha = T_{int} + \Pi_{N_{gen}} V_\alpha \Pi_{N_{gen}}$$

with projection operator $\Pi_{N_{gen}}$ on rel. HO states with $2N + L \leq N_{gen}$

**generator has explicit scale parameters**: $N_{gen}$ & $\hbar \Omega$

![Diagram showing HO matrix elements, $^1S_0$ channel, $\hbar \Omega = 24$ MeV]
### Choice of Generator: Block Generators

- **Q block generator**: use $H_\alpha$ matrix elements for states below $Q_{\text{gen}}$ and $T_{\text{int}}$ matrix elements above, i.e.,

$$G_\alpha = T_{\text{int}} + \Pi_{Q_{\text{gen}}} V_{\alpha} \Pi_{Q_{\text{gen}}}$$

with projection operator $\Pi_{Q_{\text{gen}}}$ on rel. momentum states with $q \leq Q_{\text{gen}}$

- generator has **explicit scale parameter**: $Q_{\text{gen}}$

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*momentum-space matrix elements, $^1S_0$ channel*
$^4\text{He}: \text{Convergence vs. Induced Many-Body}$

- **T$_{\text{int}}$ Generator**
- **HO-Block Generator**

- $\alpha$-dependence of block generator quickly saturates
- Block protects low-lying matrix elements from further change

\[
E_{gs} [\text{MeV}] \quad \text{vs.} \quad N_{\text{max}}
\]

- $\alpha$ [fm$^4$]:
  - 0.01
  - 0.02
  - 0.04
  - 0.0625
  - 0.08
  - 0.16

- $N_{\text{gen}} = 10$

- $\hbar\Omega = 24$ MeV
- HO basis
\textbf{\textsuperscript{4}He: Convergence vs. Induced Many-Body}

- \( N_{\text{gen}} \) controls convergence and induced many-body forces
- induced 3N appear smaller than with T\textsubscript{int} generator

**T\textsubscript{int} Generator**

- \( \alpha \) [fm\(^4\)]
  - 0.01
  - 0.02
  - 0.04
  - 0.0625
  - 0.08
  - 0.16

**HO-Block Generator**

- \( N_{\text{gen}} \)
  - 12
  - 10
  - 8
  - 6

\( \alpha = 0.0625 \text{ fm}^4 \)

\( \hbar \Omega = 24 \text{ MeV} \)

HO basis
$^4\text{He}$: Convergence vs. Induced Many-Body

- Q-block generator exhibits similar behaviour
- typical $Q_{\text{gen}} \sim 2 \text{ fm}^{-1}$

**T$_{\text{int}}$ Generator**

**Q-Block Generator**

- $E_{gs}$ [MeV] vs. $N_{\text{max}}$
  - $\alpha [\text{fm}^4]$:
    - 0.01
    - 0.02
    - 0.04
    - 0.0625
    - 0.08
    - 0.16

- $Q_{\text{gen}} [\text{fm}^{-1}]$:
  - 2.5
  - 2.2
  - 2.0
  - 1.8

- $\alpha = 0.0625 \text{ fm}^4$

- NN only
  - $\hbar \Omega = 24 \text{ MeV}$
  - HO basis
\( ^4\text{He}: \text{Efficiency Test} \)

**Dynamic Blocks**

- Efficiency test: dial same magnitude of induced 3N and compare convergence.
- Q- & HO-block give better convergence than \( T_{\text{int}} \) for same induced 3N.

**Static Blocks**

- Using static block generators \( (G_\alpha = G_0) \) gives similar results.

**Graphs**

- \( E_{gs} \) vs. \( N_{\text{max}} \)
- \( N_{\text{gen}} = 8, \alpha = 0.0625 \text{ fm}^4 \) for HO-block.
- \( Q_{\text{gen}} = 2.0 \text{ fm}^{-1}, \alpha = 0.0625 \text{ fm}^4 \) for Q-block.
- \( T_{\text{int}}: \alpha = 0.01 \text{ fm}^4 \)
- \( \hbar \Omega = 24 \text{ MeV} \) for HO basis.
### SRG Evolution in 3N

- Extension of block generators to SRG evolution in three-body space *rather* straightforward (with static generators)
- Careful with embedding and generalisation of scale definition
- First results for HO-block generator available

### Many-Body Solution

- Any many-body approach will do, i.e., not restricted to $N_{\text{max}}$ truncated NCSM space
- First results from In-Medium SRG available
- Using HF basis and including 3N contributions included in NO2B approximation
IM-SRG Results

- **NN+3N\text{\textsubscript{ind}}** agrees well for both generators: induced 4N are small as expected

- **NN+3N\text{\textsubscript{full}}** is much less bound with block generator

\[ E_{gs} \text{[MeV]} \]

\[ e_{max} \]

\[ \alpha = 0.0625 \text{ fm}^4 \]

\[ \hbar \Omega = 24 \text{ MeV} \]

\[ \Lambda_{3N} = 500 \text{ MeV} \]

\[ N_{\text{gen}} = 8 \]

\[ \Lambda_{3N} = 500 \text{ MeV} \]

\[ N_{\text{gen}} = 8 \]

\[ \alpha = 0.0625 \text{ fm}^4 \]

\[ \hbar \Omega = 24 \text{ MeV} \]

HF basis
- $E_{gs}$ vs $e_{max}$ for $^{24}O$

- $T_{int}$ Generator
- HO-Block Generator

- $NN + 3N_{ind}$ agrees well for both generators: induced 4N are small as expected

- $NN + 3N_{full}$ is much less bound with block generator

- VERY PRELIMINARY

- chiral $NN + 3N$
- $\Lambda_{3N} = 500$ MeV
- $N_{gen} = 8$
- $\alpha = 0.0625$ fm$^4$
- $\hbar\Omega = 24$ MeV
- HF basis
IM-SRG Results

- $E_{gs}$ vs $e_{max}$
- $T_{int}$ Generator vs HO-Block Generator
- $NN+3N_{ind}$ agrees well for both generators: induced 4N are small as expected
- $NN+3N_{full}$ is much less bound with block generator
- Pattern looks very promising
- Need to study $N_{gen}$ and $Q_{gen}$ dependence and do further IT-NCSM runs
Improved Chiral NN Interactions

with the LENPIC Collaboration

E. Epelbaum, H. Krebs, U.-G. Meißner, S. Binder, K. Hebeler, J. Langhammer,
J. Golak, R. Skibiński, K. Topolnicki, H. Witała, P. Maris, H. Potter, J. Vary, A. Nogga,
H. Kamada, D. Furnstahl, V. Bernard, A. Calci
Improved Chiral NN Interactions

- family of improved chiral NN interactions from LO to N4LO with (semi)local regulators  
  [talk by Hermann Krebs]
  

- matrix elements of corresponding 3N interactions up to N3LO are being generated  
  [talk by Kai Hebeler]

- initial questions from many-body perspective:
  - how do (semi)local regulators affect convergence?
  - what is the order-by-order systematics of observables and convergence?
  - uncertainty estimation from order-by-order at fixed cutoff feasible?
  - do the interactions behave well under SRG transformation?
$^4$He: Cutoff Dependence @ N3LO

\begin{center}
\includegraphics[width=\textwidth]{graph.png}
\end{center}

(semi)local interactions are somewhat harder than Entem & Machleidt

N3LO, $R = 0.9\ldots1.2$ fm

bare NN
\( ^4\text{He} \): Order-by-Order @ 1.2 fm

striking order-by-order pattern in convergence and converged energy

LO...N4LO, R = 1.2 fm bare NN

Nmax  16  14  12  10  8  6

correlated with appearance of new contacts/LECs
Epilogue

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JUROPA

LOEWE-CSC

EDISON

Computation Time