News from Ab Initio Theory

Robert Roth
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
• 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
Ab Initio Workflow

Nuclear Structure & Reaction Observables

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

- different many-body methods for different observables and mass regimes
- hot topics: continuum & open-shell medium-mass nuclei
Interactions
Chiral EFT for Nuclear Interactions

- **low-energy effective field theory** for relevant degrees of freedom \( (\pi, N) \) based on symmetries of QCD
- explicit long-range **pion dynamics**
- unresolved short-range physics absorbed in **contact terms**, low-energy constants fit to experiment
- hierarchy of **consistent NN, 3N, 4N,...** interactions and current operators
- many **ongoing developments**
  - improved NN up to N4LO
  - 3N interaction up to N3LO
  - 4N interaction at N3LO
  - improved fits and error analysis

### Standard Interaction:
- **NN @ N3LO**
  - (Entem & Machleidt, cutoff 500 MeV)
- **3N @ N2LO**
  - (local, cutoff 400 or 500 MeV)
Similarity Renormalization Group

- Continuous unitary transformation driving Hamiltonian towards diagonal form

- Unitary transformation via flow equation
  \[ H_\alpha = U_\alpha^\dagger H_0 U_\alpha \]
  \[ \frac{d}{d\alpha} H_\alpha = [\eta_\alpha, H_\alpha] \]

- Dynamic generator determines physics of transformation
  \[ \eta_\alpha = (2\mu)^2 [T_{\text{int}}, H_\alpha] \]

- Solve flow equation using matrix representation in two- and three-body space

- Flow parameter \( \alpha \) determines how far to go
Similarity Renormalization Group

**pro:**
- improves convergence of many-body calculations

**con:**
- induces many-body interactions

- need to truncate evolved Hamiltonian
  
  \[ H_\alpha = H^{[1]}_\alpha + H^{[2]}_\alpha + H^{[3]}_\alpha + H^{[4]}_\alpha + \cdots \]

- variation of flow parameter provides diagnostic for omitted many-body terms

- truncations used in the following:
  - **NN+3N\textsubscript{ind}**
    - use initial NN, keep evolved NN+3N
  - **NN+3N\textsubscript{full}**
    - use initial NN+3N, keep evolved NN+3N

Glazek, Wilson, Wegner, Perry, Bogner, Furnstahl, Hergert, Roth,...
Light Nuclei
No-Core Shell Model & Friends

NCSM-type approaches are the most powerful and universal ab initio methods for the p- and lower sd-shell

- **NCSM**: solve eigenvalue problem of Hamiltonian represented in model space of HO Slater determinants truncated w.r.t. HO excitation energy $N_{\text{max}}\hbar\Omega$
  - convergence of observables w.r.t. $N_{\text{max}}$ is the only limitation and source of uncertainty

- **Importance-Truncated NCSM**: reduce NCSM model space to physically relevant basis states and extrapolate to full space a posteriori
  - increases the range of applicability of NCSM significantly

- **NCSM with Continuum**: merge NCSM for description of clusters with Resonating Group Method for description of their relative motion
  - explicitly includes continuum degrees of freedom

- more: Gamow NCSM, Symplectic NCSM, ...
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
representing $H |\psi^{J\pi T}\rangle = E |\psi^{J\pi T}\rangle$ using the **over-complete basis**

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

expansion in $A$-body (IT-)NCSM eigenstates

leads to the **NCSMC equations**

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

with $3N$ contributions in

- $H_{\text{NCSM}}$ covered by (IT-)NCSM
- $h$ given by $\langle \Psi_A E_{\lambda'} J^{\pi T} | H |\xi^{J\pi T}_{\nu r}\rangle$
- $\mathcal{H}$ contains NCSM/RGM Hamiltonian kernel

access targets beyond $^4\text{He}$ using uncoupled densities and on-the-fly algorithm
Spectrum 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 $0^+, 2^+$ NCSM states of $^8$Be for n-$^8$Be dynamics
  • include 6 neg. and 4 pos. parity NCSM states of $^9$Be

use standard NN+3N Hamiltonian
  • NN @ N3LO, Entem & Machleidt, cutoff 500 MeV
  • 3N @ N2LO, local, cutoff 500 MeV

Langhammer et al.; PRC 91, 021301(R) (2015)
Phase Shifts for n-$^8$Be Scattering

- Negative parity phase-shifts are well converged, positive parity more difficult
- Extract resonance parameters from inflection point and derivative

$$\alpha = 0.0625 \text{ fm}^4, \ \hbar \Omega = 20 \text{ MeV}, \ E_{\text{3max}} = 14$$
$^9$Be: 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
- continuum plays more important role than chiral 3N interaction
- NCSMC predictions for widths are in fair agreement with experiment
Bridge to Medium-Mass Nuclei
Oxygen Isotopes

- **oxygen isotopic chain** has received significant attention and documents the **rapid progress** over the past years


- **2010**: **shell-model calculations** with 3N effects highlighting the role of 3N interaction for drip line physics

  Hagen, Hjorth-Jensen, Jansen, Machleidt, Papenbrock, PRL 108, 242501 (2012)

- **2012**: **coupled-cluster calculations** with phenomenological two-body correction simulating chiral 3N forces

  Hergert, Binder, Calci, Langhammer, Roth, PRL 110, 242501 (2013)

- **2013**: **ab initio IT-NCSM** with explicit chiral 3N interactions and first **multi-reference in-medium SRG** calculations...

  Cipollone, Barbieri, Navrátil, PRL 111, 062501 (2013)

  Bogner, Hergert, Holt, Schwenk, Binder, Calci, Langhammer, Roth, PRL 113, 142501 (2014)

  Jansen, Engel, Hagen, Navratil, Signoracci, PRL 113, 142502 (2014)

- since: self-consistent Green’s function, shell model with valence-space interactions from in-medium SRG or Lee-Suzuki,...
Ground States of Oxygen Isotopes

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\text{max}} = 14, \quad \text{optimal } h\Omega \]
Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

Parameter-free ab initio calculations with explicit chiral 3N interactions

Highlights predictive power of chiral NN+3N interactions

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm} \]

\[ E_{3m} = 14 \text{, optimal } \hbar \omega \]
Spectra of Oxygen Isotopes

Bogner et al., PRL 113, 142501 (2014) & Roth et al., in prep.

\[ E_x \] [MeV]

\[ N_{\text{max}} \]

\( \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad h\Omega = 16 \text{ MeV} \)

Medium-Mass Approaches

**advent of novel ab initio many-body approaches gives access to the medium-mass regime**

- **coupled-cluster theory**: ground-state parametrized by exponential wave operator applied to single-determinant reference state
  - truncation at doubles level (CCSD) plus triples correction
  - equations of motion for excited states and

- **in-medium SRG**: completely decouples particle-hole excitations from many-body reference state
  - normal-ordering evolving Hamiltonian truncated at two-body level
  - both closed- and open-shell ground states; excitations via EOM or SM

- **self-consistent Green’s function approaches and others...**

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*Hagen, Papenbrock, Dean, Piecuch, Binder,...*

*Barbieri, Soma, Duguet,...*
Ground States of Oxygen Isotopes

$NN+3N_{\text{ind}}$
(chiral NN)

$NN+3N_{\text{full}}$
(chiral NN+3N)

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08$ fm$^4$, $E_{3\text{max}} = 14$, optimal $h\Omega$

Hergert et al., PRL 110, 242501 (2013)
Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad E_{3\text{max}} = 14, \quad \text{optimal } h\Omega \]
Ground States of Oxygen Isotopes

Hergert et al., PRL 110, 242501 (2013)

\[ E_A \quad \alpha = 0.08 \text{ fm}, \alpha = 0.08 \text{ fm} \]

different many-body approaches using the same chiral NN+3N interaction give consistent results

minor differences are understood in terms of uncertainties due to truncations
Towards Heavy Nuclei - Ab Initio

CR-CC(2,3)

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04$ fm$^4$, $E_{3\text{max}} = 18$, optimal $h\Omega$
Towards Heavy Nuclei - Ab Initio

- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to $A \sim 130$
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically... redo with N2LO$_{\text{sat}}$
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \rightarrow 0.04$ fm$^4$, $E_{3\text{max}} = 18$, optimal $\hbar \Omega$
Open-Shell Medium-Mass Nuclei

- systematic MR-IM-SRG study of even Ca and Ni isotopes
- excellent agreement with best available coupled-cluster results
- chiral 3N interaction changes behavior at and beyond $^{54}$Ca

$\Lambda_{3N} = 400$ MeV
$\alpha = 0.04$ fm$^4$ (○)
$0.08$ fm$^4$ (●)
$E_{3\text{max}} = 14, 16$
Open-Shell Medium-Mass Nuclei

- two-neutron separation energies hide overall energy shift
- compares well to updated Gor'kov-GF results
  \[ \text{[priv. comm. V. Soma]} \]
- chiral 3N interaction predicts flat "drip-region" from $^{56}\text{Ca}$ to $^{60}\text{Ca}$

\[ S_{2n} \text{[MeV]} \]

$^{ACa}_{\text{Ca}}$

$\text{NN+3N}_{\text{ind}}$

(chiral NN)

$\text{NN+3N}_{\text{full}}$

(chiral NN+3N)

$a = 0.04\text{ fm}^4$ (○)

$E_{3\text{max}} = 14, 16$

$\Lambda_{3N} = 400$ MeV

$\Lambda_{3N} = 350$ MeV
News:

Merging NCSM and IM-SRG

with

Eskendr Gebrerufael, Heiko Hergert, Klaus Vobig
In-Medium SRG

- Flow equation for Hamiltonian

\[
\frac{d}{ds} H(s) = [\eta(s), H(s)]
\]

- Hamiltonian in single-reference or multi-reference (Kutzelnigg/Mukherjee) normal order, omitting normal-ordered 3B term

\[
H(s) = E(s) + \sum_{ij} f^i_j(s) \tilde{A}_j^i + \frac{1}{4} \sum_{ijkl} \Gamma_{ijkl}(s) \tilde{A}_{kl}^{ij} + \frac{1}{36} \sum_{ijklmn} W_{ijklmn}(s) \tilde{A}_{lmn}^{ijk}
\]

use SRG flow equations for normal-ordered Hamiltonian to decouple many-body reference state from excitations
IM-SRG Generators

- **Wegner**: simple, intuitive, inefficient
  \[ \eta = [H_d, H] = [H_d, H_{od}] \]

- **White**: efficient, problems with near degeneracies
  \[ \eta^1_2 = (\Delta^1_2)^{-1} n_1 \n_2 f^1_2 - [1 \leftrightarrow 2] \]
  \[ \eta^{12}_{34} = (\Delta^{12}_{34})^{-1} n_1 n_2 \n_3 \n_4 \Gamma^{12}_{34} - [12 \leftrightarrow 34] \]

- **Imaginary Time**: good work horse \([\text{Morris, Bogner}]\)
  \[ \eta^1_2 = \text{sgn}(\Delta^1_2) n_1 \n_2 f^1_2 - [1 \leftrightarrow 2] \]
  \[ \eta^{12}_{34} = \text{sgn}(\Delta^{12}_{34}) n_1 n_2 \n_3 \n_4 \Gamma^{12}_{34} - [12 \leftrightarrow 34] \]

- **Brillouin**: better work horse \([\text{Hergert}]\)
  \[ \eta^1_2 = \langle \Phi | [\tilde{A}^1_2, H] | \Phi \rangle \]
  \[ \eta^{12}_{34} = \langle \Phi | [\tilde{A}^{12}_{34}, H] | \Phi \rangle \]
## Interfaces with NCSM

### NCSM before IM-SRG
- Use ground-state from NCSM at small \( N_{\text{max}} \) as reference state for multi-reference IM-SRG
- Not limited to subsets of open-shell nuclei and systematically improvable

### NCSM after IM-SRG
- Use normal-ordered Hamiltonian \( H(s) \) at some value of the flow parameter for a subsequent NCSM or CI calculation
- Access to excited states and full spectroscopy, additional diagnostics for the ground state
- Can use the in-medium evolved Hamiltonian also in other approaches, e.g., equations-of-motion methods, RPA, Second-RPA
- This is different from IM-SRG for generating shell-model interactions
NCSM-MR-IM-SRG-NCSM Workflow

- pick interaction and nucleus
- solve NCSM problem in small $N_{\text{max}}$
- ground state defines reference state

compute density matrices and multi-ref. normal-ordered Hamiltonian

- solve MR-IM-SRG flow equations
- spherical formulation limited to scalar densities for now

extract evolved Hamiltonian in vacuum representation

- NCSM or CI calculation for ground and excited states
- ...
$^{16}\text{O}: \text{Flowing Energy}$

**Chiral NN+3N**

- $\Lambda_{3N}=500\text{ MeV}$
- $\alpha=0.08\text{ fm}^4$
- $\hbar\Omega=20\text{ MeV}$

- $N_{\text{max}}=0$
- reference state
- $e_{\text{max}}=4$
$^{12}$C: Flowing Energy

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**$^{12}$C**

- chiral NN+3N
- $\Lambda_{3N} = 500$ MeV
- $\alpha = 0.08 \text{ fm}^4$
- $\hbar \Omega = 20$ MeV
- $N_{\text{max}} = 0$
- reference state
- $e_{\text{max}} = 4$
12C: Flowing Energy

\[ E \text{ [MeV]} \]

-70
-75
-80
-85
-90
-95
-100

\[ \log s \]

-4
-3
-2
-1
0

Imaginary Time

Brillouin

12C

chiral NN+3N
\[ \Lambda_{3N}=500 \text{ MeV} \]
\[ \alpha=0.08 \text{ fm}^4 \]
\[ \hbar\Omega=20 \text{ MeV} \]

\[ N_{\text{max}}=0 \]
reference state

\[ e_{\text{max}}=4 \]

NCSM with flowing Hamiltonian

- \( N_{\text{max}}=0 \)
- \( N_{\text{max}}=2 \)
- \( N_{\text{max}}=4 \)
Oxygen Isotopes

chiral NN+3N
\[ \Lambda_{3N} = 400 \text{ MeV} \]
\[ \alpha = 0.08 \text{ fm}^4 \]
\[ \hbar \Omega = 20 \text{ MeV} \]

\[ N_{\max} = 0 \]
reference state

\[ E(s_{\min}) \]
\[ N_{\max} = 0 \]
\[ N_{\max} = 2 \]
\[ N_{\max} = 4 \]
News:

Importance Truncated Shell Model

with Christina Stumpf
importance measure for basis state $|\Phi_\nu\rangle$ for the description of target state represented by $|\Psi_{\text{ref}}\rangle$

$$
\kappa_\nu = -\frac{\langle \Phi_\nu | H | \Psi_{\text{ref}} \rangle}{\epsilon_\nu - \epsilon_{\text{ref}}}
$$

- reduce model space to important basis states with $|\kappa_\nu| \geq \kappa_{\text{min}}$ for a given importance threshold $\kappa_{\text{min}}$

- solve eigenvalue problem for a set of importance thresholds and extrapolate a posteriori to full space
Importance Truncated SM

- valence-space shell model also **limited by model-space dimension**, specifically for pf-shell and beyond or multi-shell valence spaces

- apply **importance truncation** for a sequence of $T_{\text{max}}$-truncated model spaces, analogously to $N_{\text{max}}$ sequence in NCSM

**sequential IT-SM algorithm:**

1. do full SM calculation up to convenient $T_{\text{max}}$
2. use components of eigenstates with $|C_\nu| \geq C_{\text{min}}$ to define reference states
3. consider all basis states from $T_{\text{max}} = T_{\text{max}}+2$ space and add those with $|\kappa_\nu| \geq \kappa_{\text{min}}$ to importance truncated space
4. solve eigenvalue problem in importance truncated space (for set of $\kappa_{\text{min}}$)
5. goto (2)

- in the limit $\kappa_{\text{min}}, C_{\text{min}} \to 0$ the full $T_{\text{max}}$-truncated model space is recovered
$^{56}\text{Ni}$: Threshold Dependence

$^{56}\text{Ni}$

GXPF1A

full pf space ($T_{\text{max}}=16$)

$C_{\text{min}}$

- $1 \times 10^{-4}$
- $2 \times 10^{-4}$
- $3 \times 10^{-4}$

$E - E_{\text{core}}$ [MeV]

$\kappa_{\text{min}} [10^{-5}]$

$2$ orders of magnitude

15 keV

full SM; Horoi, Brown et al; PRC 73, 061305(R) (2006)
energy variance provides a model-independent measure for the “distance” of an approximate state (truncated space) from a true eigenstate (full space)

\[ \Delta E^2 = \langle \psi | H^2 | \psi \rangle - \langle \psi | H | \psi \rangle^2 \]

- energy shows predominantly linear dependence on \( \Delta E^2 \), use quadratic term as sub-leading correction

- evaluation of expectation value of \( H^2 \) is expensive...
  - NCSM: insert completeness relation for full \( N_{\text{max}} \) space
  - SM: compute valence-space matrix elements of \( H^2 \) explicitly (up to 4B)

- was explored in NCSM and is applied routinely in MCSM calculations

$^{56}\text{Ni}$: Threshold vs. Variance

threshold dep.

variance dep.

$C_{\text{min}}$

- $1 \times 10^{-4}$
- $2 \times 10^{-4}$
- $3 \times 10^{-4}$

GXPF1A

full pf space (T$_{\text{max}}$=16)
56Ni: Threshold vs. Variance

threshold dep.

variance dep.

56Ni

GXPF1A

full pf space
(T_{\text{max}}=16)

C_{\text{min}}

- 1 \times 10^{-4}
- 2 \times 10^{-4}
- 3 \times 10^{-4}
$^{56}\text{Ni}$: Variance with $T_{\text{max}}$ Truncation

$C_{\text{min}}$ truncation

- $C_{\text{min}} = 1 \times 10^{-4}$
- $2 \times 10^{-4}$
- $3 \times 10^{-4}$

$T_{\text{max}}$ truncation

- $T_{\text{max}} = 6$
- $8$
- $10$

$E - E_{\text{core}}$ [MeV] vs. $\Delta E^2$ [MeV$^2$]

$^{56}\text{Ni}$

GXPF1A

pf space
$^{56}$Ni: Excitation Spectrum

**Threshold dependence**

- $E - E_{\text{core}}$ vs. $\kappa_{\text{min}}$ [10$^{-5}$]

**Variance dependence**

- $\Delta E^2$ vs. $\Delta E^2$ [MeV$^2$]

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$^{56}$Ni

GXPF1A

Full pf space

($T_{\text{max}}=16$)

---

**C$^{\text{min}}$**

- $1 \times 10^{-4}$
- $2 \times 10^{-4}$
- $3 \times 10^{-4}$
56Ni: Excitation Spectrum

threshold extrapolation

full SM*

variance

$\begin{align*}
5+ \\
3+ \\
4+ \\
0+ \\
2+ \\
0+
\end{align*}$

$\begin{align*}
56^{\text{Ni}}
\end{align*}$

GXPF1A

$further applications: 60^{\text{Zn}}, 64^{\text{Ge}} in pfg_{9/2} space (PFG9B3)$

* Horoi, Brown et al; PRC 73, 061305(R) (2006)
Epilogue

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COMPUTING TIME