Advances in Ab Initio Nuclear Structure Theory

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Ab Initio Nuclear Structure Theory

solve nuclear many-body problem based on realistic interactions using controlled and improvable truncations with quantified theoretical uncertainties

Interactions
- chiral effective field theory for nuclear interactions (NN+3N+...) and electroweak operators
- physics-conserving unitary transformation to adapt Hamiltonian to finite low-energy model spaces

Many-Body Method
- solve many-body Schrödinger equation numerically using only controlled truncations
- range of powerful methods for different mass ranges employing the same interaction

Quantification of Theory Uncertainties
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)

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Similarity Renormalization Group

- Continuous unitary transformation driving Hamiltonian towards diagonal form

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

- 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_{ind}**
    use initial NN, keep evolved NN+3N
  - **NN+3N_{full}**
    use initial NN+3N, keep evolved NN+3N

\[ \alpha = 0.00 \text{ fm}^4 \]

\[ \alpha = 0.16 \text{ fm}^4 \]
Many-Body Methods I:

Light Nuclei
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: Symplectic NCSM, Gamow NCSM,...
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
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

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

- Continuum plays more important role than chiral 3N interaction
- NCSMC predictions for widths are in fair agreement with experiment
Oxygen Isotopes

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

  *Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL 105, 032501 (2010)*

- **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

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)

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

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

Highlights predictive power of chiral NN+3N interactions
Spectra of Oxygen Isotopes

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

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \text{ fm}^4, \quad \hbar \Omega = 16 \text{ MeV} \]
Many-Body Methods II:
Medium-Mass Nuclei
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**: complete decoupling of particle-hole excitations from many-body reference state through SRG evolution
  - normal-ordered 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...

controlling and quantifying the uncertainties due to various inherent truncations is a major task

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

Barbieri, Soma, Duguet,...
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)

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

**Ground States of Oxygen Isotopes**

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

\[ \text{NN} + 3N \]

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

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

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

\( A_0 \)

\[ \begin{array}{c}
12 & 14 & 16 & 18 & 20 & 22 & 24 & 26 \\
-180 & -160 & -140 & -120 & -100 & -80 & -60 & -40
\end{array} \]

- 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

$\Lambda_{3N} = 400$ 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 $A \approx 130$

standard chiral NN+3N interaction overbinds medium-mass nuclei systematically

SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

$\Lambda_{3N} = 400$ MeV, $\alpha = 0.08 \to 0.04$ fm$^4$, $E_{3m\max} = 18$, optimal $h\Omega$

O $^{16}$O $^{24}$O $^{36}$Ca $^{56}$Ni $^{60}$Ni $^{62}$Ni $^{68}$Ni $^{78}$Ni $^{88}$Sr $^{100}$Sn $^{106}$Sn $^{114}$Sn $^{116}$Sn $^{120}$Sn $^{132}$Sn

CR-CC(2,3)

Binder et al., PLB 736, 119 (2014)
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 $^{54}\text{Ca}$

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

Hergert et al., PRC 90, 041302(R) (2014)

- two-neutron separation energies hide overall energy shift

- compares well to updated Gor’kov-GF results
  
  [priv. comm. V. Soma]

- chiral 3N interaction predicts flat "drip-region" from $^{56}$Ca to $^{60}$Ca

\[ A_{\text{Ca}} \]

$S_{2n}$ [MeV]

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

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

\[ A \]

- $\Lambda_{3N} = 400$ MeV
- $\Lambda_{3N} = 350$ MeV

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

$\alpha = 0.04 \text{ fm}^4$ (○)
$0.08 \text{ fm}^4$ (●)
Many-Body Methods III:

Hypernuclei
Ab Initio Hypernuclear Structure

- precise data on ground states & spectroscopy of hypernuclei
- ab initio few-body ($A \lesssim 4$) and phenomenological shell or cluster model calculations so far
- chiral YN & YY interactions at (N)LO are available

Time to transfer ab initio toolbox to hypernuclei
Application: $^7$Li

$^6$Li

$^7$Λ$^7$Li

**IT-NCSM**

NN @ N3LO
\[ \Lambda_{NN} = 500 \text{ MeV} \]
Entem&Machleidt

3N @ N2LO
\[ \Lambda_{3N} = 500 \text{ MeV} \]
Navratil
A = 3 fit

Jülich’04
Haidenbauer et al.
scatt. & hypertriton

\[ \alpha_{NN} = 0.08 \text{ fm}^4 \]
\[ \alpha_{YN} = 0.00 \text{ fm}^4 \]
\[ h\Omega = 20 \text{ MeV} \]
Application: $^7\Lambda\text{Li}$

IT-NCSM

- $^{\Lambda NN}_N$ @ N3LO
  - $\Lambda_{NN} = 500$ MeV
  - Entem&Machleidt

- $^{\Lambda 3N}_N$ @ N2LO
  - $\Lambda_{3N} = 500$ MeV
  - Navratil
  - $A = 3$ fit

- $^{\Lambda YN}_N$ @ LO
  - $\Lambda_{YN} = 600$ MeV
  - Haidenbauer et al.
  - scatt. & hypertriton

\[ \alpha_{NN} = 0.08 \text{ fm}^4 \]
\[ \alpha_{YN} = 0.00 \text{ fm}^4 \]
\[ h\Omega = 20 \text{ MeV} \]
Application: $^7\Lambda\text{Li}$

$Wirth et al., PRL 113, 192502 (2014)$

$6\text{Li}$

$7\Lambda\text{Li}$

IT-NCSM

NN @ N3LO

$\Lambda_{NN} = 500 \text{ MeV}$

Entem&Machleidt

$3\text{N} @ N2LO$

$\Lambda_{3N} = 500 \text{ MeV}$

Navratil

$A = 3 \text{ fit}$

YN @ LO

$\Lambda_{YN} = 700 \text{ MeV}$

Haidenbauer et al.

scatt. & hypertriton

$\alpha_{NN} = 0.08 \text{ fm}^4$

$\alpha_{YN} = 0.00 \text{ fm}^4$

$h\Omega = 20 \text{ MeV}$
Application: $^9\Lambda\text{Be}$

$^8\text{Be}$

$^9\Lambda\text{Be}$

$E_{[\text{MeV}]}$ vs $N_{\text{max}}$

$E_{x\text{, MeV}}$ vs $N_{\text{max}}$

$E_{[\text{MeV}]}$ vs $N_{\text{max}}$

NN @ N3LO
$\Lambda_{NN} = 500 \text{ MeV}$
Entem&Machleidt

3N @ N2LO
$\Lambda_{3N} = 500 \text{ MeV}$
Navratil
$A = 3$ fit

YN @ LO
$\Lambda_{YN} = 600 \text{ MeV}$
Haidenbauer et al.
scatt. & hypertriton

$\alpha_{NN} = 0.08 \text{ fm}^4$
$\alpha_{YN} = 0.00 \text{ fm}^4$
$h\Omega = 20 \text{ MeV}$
Application: $\Lambda^{13}\text{C}$

- Hypernuclear structure sets tight constraints on YN interaction.
- Ready to explore the physics of p-shell hypernuclei.

- $\Lambda_{NN} = 500$ MeV
  - Entem & Machleidt
- $\Lambda_{3N} = 500$ MeV
  - Navratil
  - $A = 3$ fit
- $\Lambda_{YN} = 600$ MeV
  - Haidenbauer et al.
  - scatt. & hypertriton

- $\alpha_{NN} = 0.08$ fm$^4$
- $\alpha_{YN} = 0.00$ fm$^4$
- $h\Omega = 20$ MeV

Wirth et al., PRL 113, 192502 (2014)
Conclusions
A Look Back…

- past few years have seen dramatic progress in ab initio many-body methods for nuclear structure (and reactions)
  
  ...extensions of NCSM, coupled-cluster theory, in-medium SRG, self-consistent Green's function, many-body perturbation theory,…

- a number of important developments are in progress
  
  ...spectroscopy of open-shell nuclei, derivation of valence-space interactions, broad range of observables…

- the reach of ab initio methods has grown tremendously
  
  ...medium-mass and heavy nuclei, continuum effects and reaction observables, hypernuclei…
A Look Ahead...

- for the next few years the focus will move towards improvements of the chiral interactions
  ...improved fitting strategies, consistent higher orders, systematic study of order-by-order convergence, inclusion of consistent currents,...

- rigorous quantification of theoretical uncertainties will play an important role
  ...propagation of uncertainties from chiral interaction to nuclear structure observables, full quantification of many-body uncertainties...

- lots of relevant physics predictions for NUSTAR...
Epilogue

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