Ab Initio Approaches to Light Nuclei

Lecture 4: Beyond Light Nuclei

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Overview

- **Lecture 1: Fundamentals**
  - Prelude
  - Many-Body Quantum Mechanics

- **Lecture 1’: Nuclear Hamiltonian**
  - Nuclear Interactions
  - Matrix Elements

- **Lecture 2: Correlations**
  - Two-Body Problem
  - Unitary Transformations
  - Similarity Renormalization Group

- **Lecture 3: Light Nuclei**
  - Configuration Interaction
  - No-Core Shell Model
  - Importance Truncation

- **Lecture 4: Beyond Light Nuclei**
  - Coupled-Cluster Theory
  - In-Medium Similarity Renormalization Group
Ab Initio Beyond Light Nuclei

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
  - Bogner, Tsukiyama, Schwenk, Hergert,...

- **in-medium SRG**: complete decoupling of particle-hole excitations from many-body reference
  - normal-ordered evolving \( A \)-body Hamiltonian truncated at two-body level
  - both closed- and open-shell ground states; excitations via EOM or SM
  - Barbieri, Soma, Duguet,...

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

controlling and quantifying the uncertainties due to various inherent truncations is a major task
Normal Ordering
Particle-Hole Excitations

- short-hand notation for creation and annihilation operators
  \[ a_i = a_{\alpha_i}, \quad a_i^\dagger = a_{\alpha_i}^\dagger \]

- define an A-body \textbf{reference Slater determinant}
  \[ |\Phi\rangle = |\alpha_1 \alpha_2 \ldots \alpha_A \rangle = a_1^\dagger a_2^\dagger \ldots a_A^\dagger |0\rangle \]

  and construct arbitrary Slater determinants through \textbf{particle-hole excitations}
  on top of the reference state

  \[ |\Phi^p_a\rangle = a_p^\dagger a_a |\Phi\rangle \]
  \[ |\Phi^{pq}_{ab}\rangle = a_p^\dagger a_q^\dagger a_b a_a |\Phi\rangle \]

  \[ \vdots \]

\textbf{index convention:}  \(a,b,c,\ldots\) : hole states, occupied in reference state
\(p,q,r,\ldots\) : particle states, unoccupied in reference states
\(i,j,k,\ldots\) : all states
Normal Ordering

- A string of creation and annihilation operators is in **normal order** with respect to a specific reference state, if all
  - creation operators are on the left
  - annihilation operators are on the right

- Standard particle-hole operators are normal ordered with respect to the vacuum state as reference state

\[ a_i^\dagger a_j, \quad a_i^\dagger a_j^\dagger a_l a_k, \quad a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l, \ldots \]

- **Normal-ordered product** of string of operators

\[ \{ a_n a_i^\dagger \cdots a_m a_j^\dagger \} = \text{sgn}(\pi) \ a_i^\dagger a_j^\dagger \cdots a_n a_m \]

- Defining property of a normal-ordered product: **expectation value with the reference state always vanishes**

\[ \langle \Phi | \{ \ldots \} | \Phi \rangle = 0 \]
in particle-hole formulation with respect to an **A-body reference Slater determinant** things are more complicated

<table>
<thead>
<tr>
<th>particle states</th>
<th>hole states</th>
</tr>
</thead>
<tbody>
<tr>
<td>creation operators</td>
<td>( \alpha_p^\dagger, \alpha_q^\dagger, ... )</td>
</tr>
<tr>
<td>annihilation operators</td>
<td>( \alpha_p, \alpha_q, ... )</td>
</tr>
</tbody>
</table>

redefinition of creation and annihilation operators necessary to guarantee vanishing reference expectation value

\[ \langle \Phi | \{ \ldots \} | \Phi \rangle = 0 \]

starting from an operator string in vacuum normal order one has to **reorder to arrive at reference normal order**

- “brute force” using the anticommutation relations for fermionic creation and annihilation operators
- “elegantly” using Wick’s theorem and contractions...
**Normal-Ordered Hamiltonian**

- **Second quantized Hamiltonian** in vacuum normal order

\[
H = \frac{1}{4} \sum_{ijkl} \langle ij | T_{\text{int}} + V_{NN} | kl \rangle \ a_i^\dagger a_j^\dagger a_l a_k + \quad \text{normal-ordered two-body approximation: discard residual normal-ordered three-body part}
\]

- **Normal-ordered Hamiltonian** with respect to reference state

\[
H = E + \sum_{ij} f_j^i \{ a_i^\dagger a_j \} + \frac{1}{4} \sum_{ijkl} \Gamma_{kl}^{ij} \{ a_i^\dagger a_j^\dagger a_l a_k \} + \frac{1}{36} \sum_{ijkl} W_{lmn}^{ijk} \{ a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l \}
\]

\[
E = \frac{1}{2} \sum_{ab} \langle ab | T_{\text{int}} + V_{NN} | ab \rangle + \frac{1}{6} \sum_{abc} \langle abc | V_{3N} | abc \rangle
\]

\[
f_j^i = \sum_a \langle ai | T_{\text{int}} + V_{NN} | aj \rangle + \frac{1}{2} \sum_{ab} \langle abi | V_{3N} | abj \rangle
\]

\[
\Gamma_{kl}^{ij} = \langle ij | T_{\text{int}} + V_{NN} | kl \rangle + \sum_a \langle aij | V_{3N} | akl \rangle
\]

\[
W_{lmn}^{ijk} = \langle ijk | V_{3N} | lmn \rangle
\]
Coupled-Cluster Theory
Coupled-Cluster Ansatz

- coupled-cluster ground state parametrized by exponential of particle-hole excitation operators acting on reference state

\[ |\Psi_{CC}\rangle = \exp (T) |\Phi\rangle = \exp (T_1 + T_2 + \cdots T_A) |\Phi\rangle \]

- with the n-particle-n-hole excitation operators with unknown amplitudes

\[
T_1 = \sum_{a,p} t^p_a \{ a^\dagger_p a_a \}
\]
\[
T_2 = \sum_{ab,pq} t^{pq}_{ab} \{ a^\dagger_p a^\dagger_q a_b a_a \}
\]
\[
\vdots
\]

- need to truncate the excitation operator at some small particle-hole order, defining different levels of coupled-cluster approximations

\[
T_1 \quad \text{CCS}
\]
\[
T_1 + T_2 \quad \text{CCSD}
\]
\[
T_1 + T_2 + T_3 \quad \text{CCSDT}
\]
Coupled-Cluster Equations

- insert the coupled-cluster ansatz into the \textbf{A-body Schrödinger equation} and manipulate

\[ H_{\text{int}} |\psi_{\text{CC}}\rangle = E |\psi_{\text{CC}}\rangle \quad \Rightarrow \quad \exp(-T) H_{\text{int}} \exp(T) |\Phi\rangle = E |\Phi\rangle \]

to obtain Schrödinger-like equation for a \textbf{similarity-transformed Hamiltonian}

\[ \mathcal{H} |\Phi\rangle = E |\Phi\rangle \quad \text{with} \quad \mathcal{H} = \exp(-T) H_{\text{int}} \exp(T) \]

- note: this is \textbf{not a unitary transformation} and therefore the transformed Hamiltonian is non-hermitian
  - as a result approximations will be non-variational

- similarity transformation of the Hamiltonian can be expanded in a \textbf{Baker–Campbell–Hausdorff series}, which \textbf{terminates at finite order}
  - CCSD with a two-body Hamiltonian terminates after order \( T^4 \)


CCSD Equations

- project the Schrödinger-like equation onto the reference state, 1p1h states, and 2p2h states to obtain **CCSD energy and amplitude equations**

\[
\langle \Phi | H | \Phi \rangle = E_{\text{CCSD}} \\
\langle \Phi^p_a | H | \Phi \rangle = 0 \\
\langle \Phi^p_{ab} | H | \Phi \rangle = 0
\]

- after BCH-expansion these are **coupled non-linear algebraic equations** for the amplitudes \( t^p_a, t^p_{ab} \) and the CCSD energy

- for large-scale calculations use **spherical formulation**, where particle-hole operators are coupled to \( J=0 \)

- full CCSDT is too expensive, various **non-iterative triples corrections** are being used to include triples contributions

- coupled-cluster with **explicit 3N interactions** can be done and was used to test the NO2B approximation
Coupled Cluster: Pros & Cons

**PRO**
- Much more efficient than ph-truncated CI
- Can deal with explicit 3N interaction
- Size extensive
- Very mild scaling with A

**CON**
- Not variational
- Only for closed shell nuclei *
- Other observables difficult
- Only for ground states *
- Non-hermitian Hamiltonian

* Equations of motion methods give access to near-closed-shell isotopes and excited states
In-Medium SRG
Decoupling in A-Body Space

decouple reference state from all particle-hole excited states

expectation value in reference state represents ground-state energy
In-Medium SRG

- **flow equation** for Hamiltonian

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

- Hamiltonian in single-reference or multi-reference **normal order**, omitting normal-ordered 3B term

\[
H(s) = E(s) + \sum_{ij} f^i_j(s) \{ a_i^\dagger a_j \} + \frac{1}{4} \sum_{ijkl} r_{ij}^{kl}(s) \{ a_i^\dagger a_j^\dagger a_l a_k \}
\]

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

- **Wegner**: simple, intuitive, inefficient
  \[ \eta = [H_d, H] = [H_d, H_{0d}] \]

- **White**: efficient, problems with near degeneracies
  \[ \eta_2^1 = (\Delta_2^1)^{-1} n_1 \bar{n}_2 f_2^1 - \{1 \leftrightarrow 2\} \]
  \[ \eta_{34}^{12} = (\Delta_{34}^{12})^{-1} n_1 n_2 \bar{n}_3 \bar{n}_4 \Gamma_{34}^{12} - \{12 \leftrightarrow 34\} \]

- **Imaginary Time**: good work horse [Morris, Bogner]
  \[ \eta_2^1 = \text{sgn}(\Delta_2^1) n_1 \bar{n}_2 f_2^1 - \{1 \leftrightarrow 2\} \]
  \[ \eta_{34}^{12} = \text{sgn}(\Delta_{34}^{12}) n_1 n_2 \bar{n}_3 \bar{n}_4 \Gamma_{34}^{12} - \{12 \leftrightarrow 34\} \]

- **Brillouin**: potentially better work horse [Hergert]
  \[ \eta_2^1 = \langle \Phi | [H, \{ a_1^\dagger a_2 \}] | \Phi \rangle \]
  \[ \eta_{34}^{12} = \langle \Phi | [H, \{ a_1^\dagger a_2^\dagger a_4 a_3 \}] | \Phi \rangle \]
In-Medium SRG Evolution

H. Hergert

\[ \text{Figure: Graph of } E \text{ vs. } S \text{ for } ^{40}\text{Ca}. \text{ The graph shows the energy } E \text{ and } E + \text{MBPT(2)} \text{ as a function of } S. \text{ The color map on the right shows the nuclear potential } V \text{.} \]
In-Medium SRG: Pros & Cons

**PRO**
- much more efficient than ph-truncated CI
- straight-forward extension to open-shell nuclei
- size extensive
- very mild scaling with $A$
- hermitian Hamiltonian
- easy access to other observables
- bridge to shell model

**CON**
- not variational
- NO3B needs some work
Applications for Medium-Mass Nuclei
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

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Ground States of Oxygen Isotopes

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

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

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

$A^O$
Benchmark of NO2B Approximation

Roth, et al., PRL 109, 052501 (2012); Binder et al., PRC 87, 021303(R) (2013)

**NN+3N-induced vs NN+3N-full**

- **16O**
  - $h\Omega = 20$ MeV
  - CCSD-3B ($\bigcirc$ $\bullet$ $\triangle$)
  - CCSD-NO2B ($\bigcirc$ $\circ$ $\diamond$ $\triangle$)

- **24O**
  - $h\Omega = 20$ MeV
  - CCSD-3B ($\bigcirc$ $\bullet$ $\triangle$)
  - CCSD-NO2B ($\bigcirc$ $\circ$ $\diamond$ $\triangle$)

- HF basis
  - $E_{3\text{max}} = 12$
  - $\Lambda_{3N} = 400$ MeV

1% uncertainty due to NO2B approximation

**Figure Details**
- $E^\text{3m} = 12$
- $h\Omega = 20$ MeV
- $\Lambda_{3N} = 400$ MeV
Towards Heavy Nuclei - Ab Initio

Binder et al., PLB 736, 119 (2014)

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

- 2% residual uncertainty for ground-state energies due to truncations in many-body approach up to A~130
- standard chiral NN+3N interaction overbinds medium-mass nuclei systematically; underestimates radii
- SRG-induced interactions beyond the 3N level can pose severe problems; role of chiral 4N unclear

\[ \Lambda_{3N} = 400 \text{ MeV}, \quad \alpha = 0.08 \rightarrow 0.04 \text{ fm}^4, \quad E^{\text{max}}_3 = 18, \quad \text{optimal } h\Omega \]
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$^4$ (●)

$E_{3\max} = 14, 16$
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 $^{56}\text{Ca}$ to $^{60}\text{Ca}$

all MR-IM-SRG
$\alpha = 0.04 \text{ fm}^4$ (○)
$0.08 \text{ fm}^4$ (●)
$E_{3\text{max}} = 14, 16$
Conclusions
Ab Initio Frontiers

- **ab initio theory is entering new territory...**

  - **QCD frontier**
    nuclear structure connected systematically to QCD via chiral EFT

  - **precision frontier**
    precision spectroscopy of light nuclei, including current contributions

  - **mass frontier**
    ab initio calculations up to heavy nuclei with quantified uncertainties

  - **open-shell frontier**
    extend to medium-mass open-shell nuclei and their excitation spectrum

  - **continuum frontier**
    include continuum effects and scattering observables consistently

  - **strangeness frontier**
    ab initio predictions for hyper-nuclear structure & spectroscopy

...providing a coherent theoretical framework for nuclear structure & reaction calculations
Epilogue

- thanks to my group and my collaborators

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