Part III: The Nuclear Many-Body Problem

To understand the properties of complex nuclei from first principles

Microscopic Valence-Space Interactions
Model spaces
Many-body perturbation theory (MBPT)
Calculating effective interaction
In-medium Similarity RG
Monopole part of interaction
Deficiencies of this approach

How will we approach this problem:
QCD \rightarrow \text{NN (3N) forces} \rightarrow \text{Renormalize} \rightarrow \text{“Solve” many-body problem} \rightarrow \text{Predictions}
The Nuclear Many-Body Problem

Nucleus strongly interacting many-body system – how to solve $A$-body problem?

$$H\psi_n = E_n\psi_n$$

Quasi-exact solutions only in light nuclei (GFMC, NCSM…)

**Large scale**: controlled approximations to full Schrödinger Equation

**Valence space**: diagonalize exactly with reduced number of degrees of freedom

**Medium-mass**

- Valence space
- Coupled Cluster
- In-Medium SRG
- Green’s Function

**Large scale**

- Limited range:
  - Closed shell $\pm 1$
  - Even-even
- Limited properties:
  - Ground states only
  - Some excited state

- All nuclei near closed-shell cores
- All properties:
  - Ground states
  - Excited states
  - EW transitions

Coupled Cluster
In-Medium SRG
Green’s Function
From Momentum Space to HO Basis

To this point interaction matrix elements in momentum space, partial waves

\[ \langle kK, lL | V | k'K, l'L \rangle_\alpha \]

To go to finite nuclei begin from Hamiltonian

\[ H\psi_n = (T + V)\psi_n = E_n\psi_n \]

Assume many particles in the nucleus generate a mean field \( U \):

\( U \) a one-body potential simple to solve (typically Harmonic Oscillator)

\[ H = H_0 + H_1; \quad H_0 = T + U; \quad H_1 = V - U \]

So transform from momentum space to Harmonic Oscillator Basis

\[ |nl, NL; \alpha \rangle = \int k^2 dk K^2 dK R_{nl} \left( \sqrt{2\alpha k} \right) R_{NL} \left( \sqrt{1/2\alpha K} \right) |kl, KL; \alpha \rangle \]

One more (ugly) transformation from center-of-mass to lab frame:

\[ \rightarrow \langle ab; JT | V | cd; JT \rangle \]
Valence-Space Ideas

Begin with degenerate HO levels

Problem: Can’t solve Schrödinger equation in full Hilbert space
Valence-Space Ideas

Nuclei understood as many-body system starting from closed shell, add nucleons

Unperturbed
HO spectrum

Active nucleons occupy valence space

Assume filled core

Removes degeneracy in valence space only
Valence-Space Ideas

Nuclei understood as many-body system starting from closed shell, add nucleons

Valence-space Hamiltonian derived from nuclear forces:

**Single-particle energies**

\[ H_{\text{v.s.}} = \sum_i \varepsilon_i a_i^\dagger a_i + V_{\text{v.s.}} \]

**Interaction matrix elements**
Valence-Space Philosophy

Nuclei understood as many-body system starting from closed shell, add nucleons

Valence-space Hamiltonian derived from nuclear forces:

Single-particle energies

Interaction matrix elements

\[ H_{\text{eff}} = \sum_i \varepsilon_{i_{\text{eff}}} a_i^\dagger a_i + V_{\text{eff}} \]

\[ H \psi_n = E_n \psi_n \rightarrow P H_{\text{eff}} P \psi_i = E_i P \psi_i \]

Effective valence space Hamiltonian:
Sum all excitations outside valence space

Decouple valence space from excitations
Perturbative Approach

1) Effective Hamiltonian: sum excitations outside valence space
2) Self-consistent single-particle energies

\[ \varepsilon_{\text{eff}} = a \overleftrightarrow{V} + a \overleftrightarrow{V} + \cdots \]

\[ V_{\text{eff}} = a \overleftrightarrow{V} + a \overleftrightarrow{V} + \cdots \]

\[ a \overleftrightarrow{V} + a \overleftrightarrow{V} + \cdots \]

\[ \varepsilon_{\text{eff}} \]

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

\[ 0h, 1f, 2p \]

\[ 0g, 1d, 2s \]

\[ 0f, 1p \]

\[ 0p \]

\[ 0s \]

\[ 0d_{3/2} \]

\[ 1s_{1/2} \]

\[ 0d_{5/2} \]

\[ 20 \]

\[ 40 \]

\[ 70 \]

\[ 112 \]
Perturbative Approach

1) Effective Hamiltonian: sum excitations outside valence space to \( \text{MBPT}(3) \)

2) Self-consistent single-particle energies

\[ \hat{Q} = \sum \text{excitations} \]
**Perturbative Approach**

1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)
2) Self-consistent single-particle energies
3) **Harmonic-oscillator basis** of 13-15 major shells: *converged!*

![Graphs showing single-particle energies](image-url)
Perturbative Approach

1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)
2) Self-consistent single-particle energies
3) **Harmonic-oscillator basis** of 13-15 major shells: **converged!**

![Graph 1: Energy vs Major Shells](image1)

![Graph 2: Energy vs Nhω](image2)

![Graph 3: Energy vs Nhω](image3)
Aside: G-matrix Renormalization

Standard method for softening interaction in nuclear structure for decades:

Infinite summation of ladder diagrams

Need two model spaces:

1) $M$ space in which we will want to calculate (excitations allowed in $M$)

2) Large space $Q$ in which particle excitations are allowed

To avoid double counting, can’t overlap – **matrix elements depend on $M$**
Aside: G-matrix Renormalization

Standard method for softening interaction in nuclear structure for decades:

\[ G_{ijkl}(\omega) = V_{ijkl} + \sum_{mn \in Q} V_{ijmn} \frac{Q}{\omega - \varepsilon_m - \varepsilon_n} G_{mnkl}(\omega) \]

Iterative procedure
Dependence on arbitrary starting energy!
G-matrix Renormalization

Standard method for softening interaction in nuclear structure for decades:

\[ G_{ijkl}(\omega) = V_{ijkl} + \sum_{mn \in Q} V_{ijmn} \frac{Q}{\omega - \varepsilon_m - \varepsilon_n} G_{mnkl}(\omega) \]
G-matrix Renormalization

Results of **G-matrix** renormalization vs. SRG

Removes some diagonal high-momentum components
Still large low-to-high coupling in both interactions
No indication of universality
Clear difference compared with SRG-evolved interactions!
Perturbative Approach

1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)
2) Self-consistent single-particle energies
3) **Harmonic-oscillator basis** of 13-15 major shells: converged!

Compare vs G-matrix (no sign of convergence)
Clear benefit of low-momentum interactions!
Perturbative Approach

1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)
2) Self-consistent single-particle energies
3) Harmonic-oscillator basis of 13-15 major shells
4) Nuclear forces from chiral EFT
5) Requires extended valence spaces

[Diagram showing the atomic shells and orbitals for 16O, 20Ne, 28Si, and 50Ca isotopes, with arrows indicating the transition to nonperturbative treatment of higher orbits.]
Where is the nuclear dripline?

Limits defined as last isotope with positive neutron separation energy

- Nucleons “drip” out of nucleus

Neutron dripline experimentally established to $Z=8$ (Oxygen)

<table>
<thead>
<tr>
<th>$Z=8$ Elements</th>
<th>$Z=9$ Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Neutron dripline</td>
<td>Neutron dripline</td>
</tr>
<tr>
<td>$^{16}$O</td>
<td>$^{17}$O</td>
</tr>
<tr>
<td>$^{18}$O</td>
<td>$^{19}$O</td>
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<tr>
<td>$^{20}$O</td>
<td>$^{21}$O</td>
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<td>$^{40}$O</td>
<td>$^{41}$O</td>
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<tr>
<td>$^{42}$O</td>
<td>$^{43}$O</td>
</tr>
<tr>
<td>$^{44}$O</td>
<td>$^{45}$O</td>
</tr>
</tbody>
</table>

Diagram:

- The dripline for $Z=8$ is marked at $^{16}$O.
- The dripline for $Z=9$ is marked at $^{17}$O.
- The dripline for $Z=10$ is marked at $^{18}$O.
- The dripline for $Z=11$ is marked at $^{19}$O.
- The dripline for $Z=12$ is marked at $^{20}$O.
- The dripline for $Z=13$ is marked at $^{21}$O.
- The dripline for $Z=14$ is marked at $^{22}$O.
- The dripline for $Z=15$ is marked at $^{23}$O.
- The dripline for $Z=16$ is marked at $^{24}$O.
- The dripline for $Z=17$ is marked at $^{25}$O.
- The dripline for $Z=18$ is marked at $^{26}$O.
- The dripline for $Z=19$ is marked at $^{27}$O.
- The dripline for $Z=20$ is marked at $^{28}$O.
- The dripline for $Z=21$ is marked at $^{29}$O.
- The dripline for $Z=22$ is marked at $^{30}$O.
- The dripline for $Z=23$ is marked at $^{31}$O.
- The dripline for $Z=24$ is marked at $^{32}$O.
- The dripline for $Z=25$ is marked at $^{33}$O.
- The dripline for $Z=26$ is marked at $^{34}$O.
- The dripline for $Z=27$ is marked at $^{35}$O.
- The dripline for $Z=28$ is marked at $^{36}$O.
- The dripline for $Z=29$ is marked at $^{37}$O.
- The dripline for $Z=30$ is marked at $^{38}$O.
- The dripline for $Z=31$ is marked at $^{39}$O.
- The dripline for $Z=32$ is marked at $^{40}$O.
- The dripline for $Z=33$ is marked at $^{41}$O.
- The dripline for $Z=34$ is marked at $^{42}$O.
- The dripline for $Z=35$ is marked at $^{43}$O.
- The dripline for $Z=36$ is marked at $^{44}$O.

Diagram labels:

- $^{16}$O at 1970
- $^{17}$O at 1999
- $^{18}$O at 2002
- $^{19}$O at 2007
Where is the nuclear dripline?
Limits defined as last isotope with positive neutron separation energy
- Nucleons “drip” out of nucleus
Neutron dripline experimentally established to $Z=8$ (Oxygen)

Regular dripline trend… except oxygen
Adding one proton binds 6 additional neutrons
Limits of Nuclear Existence: Oxygen Anomaly

Where is the nuclear dripline?
Limits defined as last isotope with positive neutron separation energy
- Nucleons “drip” out of nucleus

Neutron dripline experimentally established to $Z=8$ (Oxygen)

Microscopic picture: **NN-forces too attractive**
Incorrect prediction of dripline
Monopole Part of Valence-Space Interactions

**Microscopic MBPT** – effective interaction in chosen model space

Works near closed shells: deteriorates beyond this

Deficiencies improved adjusting particular two-body matrix elements

**Monopoles:**
Angular average of interaction

\[ V_{ab}^T = \frac{\sum J (2J + 1) V_{abab}^{JT}}{\sum J (2J + 1)} \]

Determines interaction of orbit \( a \) with \( b \): evolution of orbital energies

\[ \Delta \varepsilon_a = V_{ab} n_b \]

Microscopic low-momentum interactions

Phenomenological USD interactions

Clear shifts in low-lying orbitals:
- \( T=1 \) repulsive shift
Physics in Oxygen Isotopes

Calculate evolution of $sd$-orbital energies from interactions

Microscopic NN Theories
$d_{3/2}$ orbit bound to $^{28}$O

Phenomenological Models
$d_{3/2}$ orbit unbound
Physics in Oxygen Isotopes

Calculate evolution of $sd$-orbital energies from interactions

**Microscopic NN Theories**
- $d_{3/2}$ orbit bound to $^{28}\text{O}$
- Dripline at $^{28}\text{O}$
- Oxygen anomaly unexplained with NN forces

**Phenomenological Models**
- $d_{3/2}$ orbit unbound
- Dripline at $^{24}\text{O}$

Origin of monopole shifts: Neglected 3N forces

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See lecture of A. Poves
**Perturbative Approach**

1) Effective Hamiltonian: sum excitations outside valence space to MBPT(3)
2) Self-consistent single-particle energies
3) Harmonic-oscillator basis of 13-15 major shells
4) Nuclear forces from chiral EFT
5) Requires extended valence spaces

**Limitations**

- Uncertain perturbative convergence
- Core physics inconsistent or absent
- Degenerate valence space requires HO basis (HF requires nontrivial extension)
- Must treat additional orbitals nonperturbatively (extend valence space)
Particle/Hole Excitations

Consider basis states as excitations from some reference state:

Reference: Slater Determinant

- 1p-1h excitation
- 2p-2h excitation

Hamiltonian schematically given in terms of ph excitations:

\[
|\Phi\rangle = \prod_{i=1}^{N} a_i^\dagger |0\rangle \\
|\Phi_i^a\rangle = a_a^\dagger a_i |\Phi\rangle \\
|\Phi_{ij}^{ab}\rangle = a_a^\dagger a_i a_b^\dagger a_j |\Phi\rangle
\]
Normal-Ordered Hamiltonian

Now rewrite exactly the initial Hamiltonian in normal-ordered form

\[ H_{\text{N.O.}} = E_0 + \sum_{ij} f_{ij} \{ a_i^\dagger a_j \} + \frac{1}{4} \sum_{jkl} \Gamma_{ijkl} \{ a_i^\dagger a_j^\dagger a_l a_k \} + \frac{1}{36} \sum_{ijklmn} W_{ijklmn} \{ a_i^\dagger a_j^\dagger a_k^\dagger a_l a_m a_n \} \]

Normal-ordered Hamiltonian w.r.t. reference state

Loop = sum over occupied states

Include dominant 1-, 2-, 3-body physics in NO
Nonperturbative In-Medium SRG

Tsukiyama, Bogner, Schwenk, PRL (2011)

In-Medium SRG continuous unitary trans. drives off-diagonal physics to zero

\[ H(s) = U(s) H U^\dagger(s) \equiv H^d(s) + H^{od}(s) \rightarrow H^d(\infty) \]

From uncorrelated Hartree-Fock reference state (e.g., \(^{16}\text{O}\)) define:

\[ H^{od} = \langle p|H|h \rangle + \langle pp|H|hh \rangle + \cdots + \text{h.c.} \]

\[ \langle i|H|j \rangle \]

\[ \langle npnh|H(\infty)|\Phi_{\text{core}} \rangle = 0 \]

Drives all n-particle n-hole couplings to 0 – **decouples** core from excitations
Define $U(s)$ implicitly from particular choice of generator:

$$\eta(s) \equiv (\frac{dU(s)}{ds}) U^\dagger(s)$$

chosen for desired decoupling behavior – e.g.,

$$\eta_I(s) = [H^d(s), H^{od}(s)] \quad \text{Wegner (1994)}$$

Solve **flow equation** for Hamiltonian (coupled DEs for 0, 1, 2-body parts)

$$\frac{dH(s)}{ds} = [\eta(s), H(s)] \quad H(s) = E_0(s) + f(s) + \Gamma(s) + \cdots$$

Hamiltonian and generator truncated at 2-body level: **IM-SRG(2)**

0-body flow drives uncorrelated ref. state to fully correlated ground state

$$E_0(\infty) \rightarrow \text{Core Energy}$$

Ab initio method for energies of **closed-shell systems**
**IM-SRG: Valence-Space Hamiltonians**

Tsukiyama, Bogner, Schwenk, PRC (2012)

**Open-shell systems**

Separate \( p \) states into valence states (\( v \)) and those above valence space (\( q \))

Redefine \( H^{od} \) to **decouple valence space from excitations** outside \( v \)

\[
H^{od} = \langle p|H|h \rangle + \langle pp|H|hh \rangle + \langle v|H|q \rangle + \langle pq|H|vv \rangle + \langle pp|H|hv \rangle + \text{h.c.}
\]

\( E_0(\infty) \rightarrow \text{Core Energy} \quad f(\infty) \rightarrow \text{SPEs} \quad \Gamma(\infty) \rightarrow V_{\text{eff}} \)
Open-shell systems

Separate $p$ states into valence states ($v$) and those above valence space ($q$)

Core physics included consistently (absolute energies, radii…)

Inherently nonperturbative – no need for extended valence space

Non-degenerate valence-space orbitals

**IM-SRG: Valence-Space Hamiltonians**

Tsukiyama, Bogner, Schwenk, PRC (2012)

### Valence Space Decoupling

- Construct generator from off-diagonal Hamiltonian

$$H(s = 0) \rightarrow H(\infty)$$
NN-only IM-SRG Monopoles

Testing ab initio IM-SRG shell model monopoles

**Monopoles:**
Angular average of interaction

Determines interaction of orbit \( a \) with \( b \): *evolution of orbital energies*

\[
V_{ab}^T = \frac{\sum J (2J + 1)V_{abab}^{JT}}{\sum J (2J + 1)}
\]

\[
\Delta \varepsilon_a = V_{ab} n_b
\]

**Improvements over MBPT?**

NN-only significantly too attractive

**NN+3N-ind** improved but \( d_{3/2} \) monopoles too attractive
Comparison with Large-Space Methods

Results from SRG-evolved NN and NN+3N-ind forces

Dripline still not reproduced
Comparison with Large-Space Methods

Large-space methods with **same SRG-evolved NN+3N-ind forces**

Agreement between all methods with same input forces

No reproduction of dripline in any case