Nuclear Structure with Similarity-Transformed Chiral NN+3N Interactions

Angelo Calci
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Outline

- Introduction
- Chiral Effective Field Theory (χEFT)
- Similarity Renormalization Group
- Transformation to $\mathcal{J}, T$-Coupled Scheme
- Importance Truncated No-Core Shell Model
- Hartree Fock
- Summary and Outlook
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start with many-body eigenvalue problem

\[ H_{\text{int}} |\psi_n\rangle = E_n |\psi_n\rangle \]

**ab-initio methods**

- investigation and adjustment of interaction
- reference point for approximative approaches
- make predictions in low-mass regime

observables to experiment
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■ Hartree Fock

■ Summary and Outlook
want to obtain an interaction based on QCD as much as possible

Quantum Chromodynamics (QCD)

- fundamental theory of the strong interaction
- uses quarks and gluons as degrees of freedom
- currently no direct derivation of nuclear interaction (non-perturbative for low-energy regime)
- effective field theory necessary

Chiral Effective Field Theory ($\chi$EFT)

- considers fundamental symmetries of QCD
- uses nucleons and pions as degrees of freedom
- perturbative expansion in $\frac{Q}{\Lambda_{\chi}}$
Expansion in $\mathcal{Q}/\Lambda_{\chi}$

<table>
<thead>
<tr>
<th>LO</th>
<th>NLO</th>
<th>N^2LO</th>
<th>N^3LO</th>
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<td>$\mathcal{Q}/\Lambda_{\chi}^0$</td>
<td>$\mathcal{Q}/\Lambda_{\chi}^2$</td>
<td>$\mathcal{Q}/\Lambda_{\chi}^3$</td>
<td>$\mathcal{Q}/\Lambda_{\chi}^4$</td>
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- **2N force**
- **3N force**
- **4N force**

- **NN interaction at $N^3$LO**
  - fitted to two-body systems
  - reproduce scattering data with high precision

- **3N interaction at $N^2$LO**

- Provides **NN and 3N interactions** in a **consistent** manner
3N Contribution at N^2LO

\[ \begin{align*}
&\sim c_D \\
&\sim c_E \\
&\sim c_1, c_3, c_4
\end{align*} \]

one-pion exchange

two-nucleon exchange

required model space for (IT)-NCSM to large to obtain converged results

\[ \Rightarrow \text{apply unitary transformation to accelerate convergence} \]

- \( c_1, c_3, c_4 \) fixed by

- new LECs of 3N interaction are \( c_D \) and \( c_E \)
  - fitted to binding energy and \( \beta \)-decay half-life of triton

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accelerate convergence by **pre-diagonalizing** the Hamiltonian w.r.t. the many-body basis

- continuous **unitary transformation** of the Hamiltonian

\[
\tilde{H}_\alpha = U_\alpha \dagger H_{\text{int}} U_\alpha
\]

- leads to **evolution equation**

\[
\frac{d}{d\alpha} \tilde{H}_\alpha = [\eta_\alpha, \tilde{H}_\alpha] \quad \text{with} \quad \eta_\alpha = -U_\alpha \dagger \frac{dU_\alpha}{d\alpha} = -\eta_\alpha^\dagger
\]

initial value problem with \( \tilde{H}_{\alpha=0} = H_{\text{int}} \)

- choose the **dynamic generator**

\[
\eta_\alpha = (2\mu)^2 [T_{\text{int}}, \tilde{H}_\alpha]
\]

advantages of SRG: **simplicity** and **flexibility**
“relative coordinates” for $A$-body system

\[
\begin{align*}
\xi_0 &= \sqrt{\frac{1}{A}} [\mathbf{r}_1 + \mathbf{r}_2 + \ldots + \mathbf{r}_A] \\
\xi_{n-1} &= \sqrt{\frac{n-1}{n}} \left[ \frac{1}{n-1} (\mathbf{r}_1 + \mathbf{r}_2 + \ldots + \mathbf{r}_{n-1}) - \mathbf{r}_n \right] \quad \text{with} \quad 2 \leq n \leq A
\end{align*}
\]

for example $A = 3$:

\[
\begin{align*}
\xi_0 &= \sqrt{\frac{1}{3}} [\mathbf{r}_1 + \mathbf{r}_2 + \mathbf{r}_3] \\
\xi_1 &= \sqrt{\frac{1}{2}} [\mathbf{r}_1 - \mathbf{r}_2] \\
\xi_2 &= \sqrt{\frac{2}{3}} \left[ \frac{1}{2} (\mathbf{r}_1 + \mathbf{r}_2) - \mathbf{r}_3 \right]
\end{align*}
\]
Insertion: HO Jacobi Basis

■ Cartesian HO state

\[ |n_1 l_1 m_1(r_1), n_2 l_2 m_2(r_2), n_3 l_3 m_3(r_3) \rangle \]

where

- \( l_1 \): quantum number w.r.t. \( \vec{L}_1 = \vec{r}_1 \times \vec{p}_1 \)
- \( l_2 \): quantum number w.r.t. \( \vec{L}_2 = \vec{r}_2 \times \vec{p}_2 \)
- \( l_3 \): quantum number w.r.t. \( \vec{L}_3 = \vec{r}_3 \times \vec{p}_3 \)

■ Jacobi HO state

\[ |NLM(\xi_0), n_{12} l_{12} m_{12}(\xi_1), N_3 L_3 M_3(\xi_2) \rangle \]

where

- \( L \): quantum number w.r.t. \( \vec{L} = \vec{\xi}_0 \times \vec{\pi}_0 \)
- \( L_3 \): quantum number w.r.t. \( \vec{L}_3 = \vec{\xi}_1 \times \vec{\pi}_1 \)

HO basis separates into the relevant intrinsic and the center of mass part.
SRG Evolution in Two-Body Space

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

\[ \Lambda = \infty \text{ fm}^{-1} \]

\[ \langle E'(L'S)J^\pi T | \hat{H}_\alpha | E(LS)J^\pi T \rangle \]

\[ J^\pi = 1^+, T = 0, \hbar \Omega = 20 \text{ MeV} \]

2B-Jacobi HO matrix elements

\[ E \to E' \to 16 \to 24 \to 32 \to 40 \]

\[ (E', i') \]

[MeV]

momentum space \[ ^3S_1 \]
SRG Evolution in Two-Body Space

\[ \alpha = 0.32 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]

\[ \langle E'(L'S)J^\pi T | \tilde{H}_\alpha | E(LS)J^\pi T \rangle \]
\[ J^\pi = 1^+, T = 0, \hbar \Omega = 20 \text{ MeV} \]

pre-diagonalization in momentum space and in HO basis

2B-Jacobi HO matrix elements

\[ (E, i) \]
\[ (E', i') \]

momentum space \[ ^3S_1 \]
3B-Jacobi HO matrix elements

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

\[ \Lambda = \infty \text{ fm}^{-1} \]

\[ \langle E' i' JT | \tilde{H}_\alpha | E iT \rangle \]

\[ J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 20 \text{ MeV} \]

NCSM ground state \(^3\text{H}\)
\[ \alpha = 0.32 \text{ fm}^4 \]
\[ \Lambda = 1.33 \text{ fm}^{-1} \]
\[ \langle E' i' JT \big| \tilde{H}_\alpha \big| E i T \rangle \]
\[ J^\pi = \frac{1}{2}^+, T = \frac{1}{2}, \hbar \Omega = 20 \text{ MeV} \]

- Pre-diagonalization of Hamiltonian
- Acceleration of convergence in many-body calculations

NCSM ground state \(^3\text{H}\)
Consideration of Induced Contributions

- **SRG induces irreducible** many-body contributions

\[
\tilde{H}_{\alpha}^{\text{NN+3N}} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int},\alpha} + \tilde{V}^{[2]}_{\text{NN},\alpha} + \tilde{T}^{[3]}_{\text{int},\alpha} + \tilde{V}^{[3]}_{\text{NN},\alpha} + \tilde{V}^{[3]}_{\text{NN},\alpha} + \tilde{T}^{[4]}_{\text{int},\alpha} + \tilde{V}^{[4]}_{\text{NN},\alpha} + \tilde{V}^{[4]}_{\text{NN},\alpha} + \ldots
\]

- **NN only**: start with NN initial Hamiltonian and evolve in two-body space

\[
\tilde{H}_{\alpha}^{\text{NN-only}} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int},\alpha} + \tilde{V}^{[2]}_{\text{NN},\alpha}
\]

- **NN+3N-induced**: start with NN initial Hamiltonian and evolve in three-body space

\[
\tilde{H}_{\alpha}^{\text{NN+3N-induced}} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int},\alpha} + \tilde{V}^{[2]}_{\text{NN},\alpha}
\]

- **NN+3N-full**: start with NN+3N initial Hamiltonian and evolve in three-body space

\[
\tilde{H}_{\alpha}^{\text{NN+3N-full}} = T_{\text{int}} + \tilde{T}^{[2]}_{\text{int},\alpha} + \tilde{V}^{[2]}_{\text{NN},\alpha} + \tilde{T}^{[3]}_{\text{int},\alpha} + \tilde{V}^{[3]}_{\text{NN},\alpha} + \tilde{V}^{[3]}_{\text{NN},\alpha} + \tilde{T}^{[4]}_{\text{int},\alpha} + \tilde{V}^{[4]}_{\text{NN},\alpha} + \tilde{V}^{[4]}_{\text{NN},\alpha} + \ldots
\]

\(\alpha\)-variation provides a diagnostic tool to assess the contributions of omitted many-body interactions.
From Jacobi to $JT$-coupled Scheme

**effective interaction in 3B-Jacobi basis**

1. **problem**
   many-body calculations ($A > 6$) in Jacobi coordinates not feasible
   → advantageous to use *$m$-scheme*

2. **problem**
   $m$-scheme matrix elements become intractable for $N_{\text{max}} > 8$ (p-shell)

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**Transformation from Jacobi into $JT$-coupled scheme**

*key for efficient application up to $N_{\text{max}} = 14$ for p-shell nuclei*

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**Ab-initio many-body calculation**
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No-Core Schalenmodell (NCSM)

- **solving the eigenvalue problem**
  \[ H_{\text{int}} |\psi_n\rangle = E_n |\psi_n\rangle \]

- **many-body basis**: Slater determinants \(|\Phi_\nu\rangle\) composed of harmonic oscillator single-particle states (m-scheme)
  \[ |\psi_n\rangle = \sum_\nu C^n_\nu |\Phi_\nu\rangle \]

- **model space**: spanned by m-scheme states \(|\Phi_\nu\rangle\) with unperturbed excitation energy of up to \(N_{\text{max}} \hbar \Omega\)

**problem**

enormous increase of model space with particle number \(A\)
\[ \Rightarrow \] converged calculation limited to small \(A\)
start with approximation $|\Psi_{\text{ref}}\rangle$ for the target state obtained in a limited reference space $\mathcal{M}_{\text{ref}}$

$$|\Psi_{\text{ref}}\rangle = \sum_{\nu \in \mathcal{M}_{\text{ref}}} C_{\nu}^{(\text{ref})} |\Phi_{\nu}\rangle$$

measure the importance of individual basis state $|\Phi_{\nu}\rangle \notin \mathcal{M}_{\text{ref}}$ via first-order multiconfigurational perturbation theory

construct importance truncated space $\mathcal{M}(\kappa_{\text{min}})$ spanned by basis states with $|\kappa_{\nu}| \geq \kappa_{\text{min}}$

solve eigenvalue problem in importance truncated space $\mathcal{M}(\kappa_{\text{min}})$ and obtain improved approximation of target state
Importance Truncation: Iterative Scheme

- **sequential calculation** for a range of $N_{\text{max}}\hbar\Omega$ spaces:
  - ✷ full NCSM calculation for small $N_{\text{max}}$ to obtain initial $|\Psi_{\text{ref}}\rangle$
  - ① construct importance-truncated space with $N_{\text{max}} + 2$ of states with $|\kappa_\nu| \geq \kappa_{\text{min}}$
  - ② solve eigenvalue problem
  - ③ use eigenstate as new $|\Psi_{\text{ref}}\rangle$
  - ④ goto ①

- **full NCSM space is recovered** in the limit $\kappa_{\text{min}} \rightarrow 0$
Threshold Extrapolation

- do calculations for a sequence of importance thresholds $\kappa_{\text{min}}$
- observables show smooth threshold dependence
- systematic approach to the full NCSM limit
- use a posteriori extrapolation $\kappa_{\text{min}} \rightarrow 0$ of observables to account for effect of excluded configurations
\( ^4\text{He}: \text{Ground-State Energies} \)

**NN only**
- strong \( \alpha \)-dependence: induced 3N interactions
- \( \hbar \Omega = 20 \text{ MeV} \)

**NN+3N-induced**
- no \( \alpha \)-dependence: no induced 4N interactions

**NN+3N-full**
- no \( \alpha \)-dependence: no induced 4N interactions

\[
\begin{align*}
\alpha &= 0.04 \text{ fm}^4 \\
\Lambda &= 2.24 \text{ fm}^{-1}
\end{align*}
\]

\[
\begin{align*}
\alpha &= 0.05 \text{ fm}^4 \\
\Lambda &= 2.11 \text{ fm}^{-1}
\end{align*}
\]

\[
\begin{align*}
\alpha &= 0.0625 \text{ fm}^4 \\
\Lambda &= 2.00 \text{ fm}^{-1}
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\[
\begin{align*}
\alpha &= 0.08 \text{ fm}^4 \\
\Lambda &= 1.88 \text{ fm}^{-1}
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\]

\[
\begin{align*}
\alpha &= 0.16 \text{ fm}^4 \\
\Lambda &= 1.58 \text{ fm}^{-1}
\end{align*}
\]
$^6\text{Li}$: Ground-State Energies

**NN only**

- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$

**NN+3N-induced**

- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$

**NN+3N-full**

- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$

$\hbar \Omega = 20 \text{ MeV}$
$^{12}\text{C}$: Ground-State Energies

**NN only**
- \( \hbar \Omega = 20 \text{ MeV} \)

**NN+3N-induced**
- no \( \alpha \)-dependence: no induced 4N contrib.

**NN+3N-full**
- some \( \alpha \)-dependence: induced 4N interactions

- \( \alpha = 0.04 \text{ fm}^4 \)
  - \( \Lambda = 2.24 \text{ fm}^{-1} \)
- \( \alpha = 0.05 \text{ fm}^4 \)
  - \( \Lambda = 2.11 \text{ fm}^{-1} \)
- \( \alpha = 0.0625 \text{ fm}^4 \)
  - \( \Lambda = 2.00 \text{ fm}^{-1} \)
- \( \alpha = 0.08 \text{ fm}^4 \)
  - \( \Lambda = 1.88 \text{ fm}^{-1} \)
- \( \alpha = 0.16 \text{ fm}^4 \)
  - \( \Lambda = 1.58 \text{ fm}^{-1} \)
\(16^O: \text{Ground-State Energies}\)

**NN only**

- \(\alpha = 0.04 \text{ fm}^4, \Lambda = 2.24 \text{ fm}^{-1}\)
- \(\alpha = 0.05 \text{ fm}^4, \Lambda = 2.11 \text{ fm}^{-1}\)

**NN+3N-induced**

- \(\alpha = 0.0625 \text{ fm}^4, \Lambda = 2.00 \text{ fm}^{-1}\)
- \(\alpha = 0.08 \text{ fm}^4, \Lambda = 1.88 \text{ fm}^{-1}\)
- \(\alpha = 0.16 \text{ fm}^4, \Lambda = 1.58 \text{ fm}^{-1}\)

**NN+3N-full**

- \(\alpha = 0.04 \text{ fm}^4, \Lambda = 2.24 \text{ fm}^{-1}\)
- \(\alpha = 0.05 \text{ fm}^4, \Lambda = 2.11 \text{ fm}^{-1}\)

- **No \(\alpha\)-dependence:**
  - No induced 4N contributions.

- **Sizable \(\alpha\)-dependence:**
  - Induced 4N interactions

\(\hbar \Omega = 20 \text{ MeV}\)
$^{16}\text{O}$ & $^4\text{He}$: Energy vs. Flow Parameter

$E_\infty$ [MeV]

$\hbar\Omega = 20$ MeV

 NN only  ■ NN+3N-induced  ▲ NN+3N-full
$^6\text{Li}$: Excitation Energies

- **NN only**
  - $\alpha = 0.04 \text{ fm}^4$
  - $\Lambda = 2.24 \text{ fm}^{-1}$

- **NN+3N-induced**
  - $\alpha = 0.05 \text{ fm}^4$
  - $\Lambda = 2.11 \text{ fm}^{-1}$

- **NN+3N-full**
  - $\alpha = 0.0625 \text{ fm}^4$
  - $\Lambda = 2.00 \text{ fm}^{-1}$

- **0+**
- **3+**
$^{12}\text{C}: \text{Excitation Energies}$

\[\hbar \Omega = 20 \text{ MeV}\]

**NN only**

- $N_{\text{max}}$
- $E_x$ [MeV]

- $\alpha = 0.04 \text{ fm}^4$
- $\Lambda = 2.24 \text{ fm}^{-1}$

**NN+3N-induced**

- $N_{\text{max}}$
- $E_x$ [MeV]

- $\alpha = 0.05 \text{ fm}^4$
- $\Lambda = 2.11 \text{ fm}^{-1}$

**NN+3N-full**

- $N_{\text{max}}$
- $E_x$ [MeV]

- $\alpha = 0.0625 \text{ fm}^4$
- $\Lambda = 2.00 \text{ fm}^{-1}$

- $\alpha = 0.08 \text{ fm}^4$
- $\Lambda = 1.88 \text{ fm}^{-1}$

- $\alpha = 0.16 \text{ fm}^4$
- $\Lambda = 1.58 \text{ fm}^{-1}$
IT-NCSM gives access to complete spectroscopy of p- and sd-shell nuclei starting from chiral NN+3N interactions.
Spectroscopy of $^{16}$C

IT-NCSM gives access to complete spectroscopy of p- and sd-shell nuclei starting from chiral NN+3N interactions.
Origin of Induced 4N Contributions

- almost same α-dependence for standard LECs and $c_D = 0$ or $c_E = 0$

⇒ two-pion exchange $(c_i)$ term induces significant many-body contributions

\[
\begin{align*}
\alpha &= 0.08 \text{ fm}^4 & \Lambda &= 1.88 \text{ fm}^{-1} \\
\alpha &= 0.16 \text{ fm}^4 & \Lambda &= 1.58 \text{ fm}^{-1}
\end{align*}
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**Hartree Fock**

- Summary and Outlook
Systematics: $E/A$ and $R_{\text{ch}}$

NN-only

$E/A$ [MeV]

$R_{\text{ch}}$ [fm]

$\alpha = 0.02 \text{ fm}^4$

$\alpha = 0.04 \text{ fm}^4$

$\alpha = 0.08 \text{ fm}^4$

$e_{\text{max}} = 14$

$E_{3,\text{max}} = 12$

$\hbar \Omega = 28 \text{ MeV}$
Systematics: E/A and $R_{ch}$

**Graph**

- **NN-only**
  - $E/A$ [MeV]
  - $R_{ch}$ [fm]
  - $\alpha = 0.02$ fm$^4$
  - $\alpha = 0.04$ fm$^4$
  - $\alpha = 0.08$ fm$^4$

- **HF + PT**
- **HF**

**Species**

- $^4$He, $^{16}$O, $^{24}$O, $^{34}$Si, $^{40}$Ca, $^{44}$Ca, $^{48}$Ni, $^{56}$Ni, $^{60}$Ni, $^{78}$Sr, $^{88}$Sr, $^{90}$Zr, $^{100}$Sn, $^{114}$Sn, $^{132}$Sn, $^{146}$Sn, $^{208}$Pb

**Equations**

- $e_{\text{max}} = 14$
- $E_{3, \text{max}} = 12$
- $\hbar \Omega = 28$ MeV

**Graph Details**

- $\alpha$ values for $R_{ch}$
- $e_{\text{max}}$ and $E_{3, \text{max}}$ for $e$-values
- $\hbar \Omega$ for energy values
Systematics: E/A and $R_{ch}$

NN + 3N-induced

- $\alpha = 0.02$ fm$^4$
- $\alpha = 0.04$ fm$^4$
- $\alpha = 0.08$ fm$^4$

$e_{max} = 14$
$E_{3,max} = 12$
$\hbar\Omega = 28$ MeV
Systematics: E/A and $R_{ch}$

**NN + 3N-induced**

### HF + PT

<table>
<thead>
<tr>
<th>Element</th>
<th>$E/A$ [MeV]</th>
<th>$R_{ch}$ [fm]</th>
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<tbody>
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<td>$^4$He</td>
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### HF

- $\alpha = 0.02\, fm^4$
- $\alpha = 0.04\, fm^4$
- $\alpha = 0.08\, fm^4$

$e_{max} = 14$

$E_{3,max} = 12$

$\hbar\Omega = 28\, MeV$

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Systematics: $E/A$ and $R_{ch}$

**Graph: NN + 3N-full**

- $E/A$ [MeV]
- $R_{ch}$ [fm]

- **HF**
- **α = 0.02 fm$^4$**
- **α = 0.04 fm$^4$**
- **α = 0.08 fm$^4$**

- Experiment

- $e_{\text{max}} = 14$
- $E_{3,\text{max}} = 12$
- $\hbar \Omega = 28$ MeV

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Systematics: E/A and $R_{ch}$

NN + 3N-full

$E/A$ [MeV]

$R_{ch}$ [fm]

strong $\alpha$-dependence: induced 4N contributions are sizable

$\alpha = 0.02 \text{ fm}^4$

$\alpha = 0.04 \text{ fm}^4$

$\alpha = 0.08 \text{ fm}^4$

experiment

$e_{\text{max}} = 14$

$E_{3,\text{max}} = 12$

$\hbar \Omega = 28 \text{ MeV}$

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Summary and Outlook
Benchmark of chiral NN+3N interactions

- consistent SRG evolution in 3B space
- efficient transformation of Jacobi matrix elements to $\mathcal{J}T$-coupled scheme
  - key for application to $N_{\text{max}} > 8$ calculations (p-shell)
- IT-NCSM with full chiral 3N interactions up to $N_{\text{max}} = 12 \ (14)$ for all p-shell (and lower sd-shell) nuclei
- two-pion exchange term of 3N interaction induces significant 4N contributions beyond mid-p-shell
  - modify SRG generator to prevent induced 4N contributions from the beginning
- many other applications (Hartree Fock, RPA, ...)

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Epilogue

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**Thank you for your attention!**