NCSM and neutrinoless double beta decay  
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The Overarching Questions
- How did visible matter come into being and how does it evolve?
- How does subatomic matter organize itself and what phenomena emerge?
- Are the fundamental interactions that are basic to the structure of matter fully understood?
- How can the knowledge and technological progress provided by nuclear physics best be used to benefit society?
  - *NRC Decadal Study*

The Time Scale
- Protons and neutrons formed $10^{-6}$ to 1 second after Big Bang (13.7 billion years ago)
- H, D, He, Li, Be, B formed 3-20 minutes after Big Bang
- Other elements born over the next 13.7 billion years
Sources of observables’ uncertainties with Chiral EFT

Working with Chiral EFT operators – uncertainties due to:

- Fitting of LECs, NN data error propagation (other LENPIC teams)
- Choice of regulator (results here for $R = 1.0$ fm)
- Truncation at a fixed Chiral order
- Numerical uncertainty at fixed $[N_{\text{max}}, hw]$ ($\sim 1$ keV in total gs energy)
- Extrapolation uncertainty (new results for gs energies)
- Other approximations, if adopted, such as normal ordering approximation, importance truncation, . . .

Working with NCSM using OLS – uncertainties due to:

- Truncation vs OLS applied to the operators
- Rank of OLS-derived operator truncation (2-body, 3-body, . . .)
No-Core Configuration Interaction calculations


Given a Hamiltonian operator

$$\hat{H} = \sum_{i<j} \frac{(\vec{p}_i - \vec{p}_j)^2}{2 mA} + \sum_{i<j} V_{ij} + \sum_{i<j<k} V_{ijk} + \ldots$$

solve the eigenvalue problem for wavefunction of $A$ nucleons

$$\hat{H} \Psi(r_1, \ldots, r_A) = \lambda \Psi(r_1, \ldots, r_A)$$

- Expand eigenstates in basis states $|\Psi\rangle = \sum a_i |\Phi_i\rangle$
- Diagonalize Hamiltonian matrix $H_{ij} = \langle \Phi_j | \hat{H} | \Phi_i \rangle$
- No-Core CI: all $A$ nucleons are treated the same
- Complete basis $\rightarrow$ exact result
- In practice
  - truncate basis
  - study behavior of observables as function of truncation

Progress in Ab Initio Techniques in Nuclear Physics, Feb. 2015, TRIUMF, Vancouver – p. 2/50
Basis expansion $\Psi(r_1, \ldots, r_A) = \sum a_i \Phi_i(r_1, \ldots, r_A)$

- Many-Body basis states $\Phi_i(r_1, \ldots, r_A)$ Slater Determinants
- Single-Particle basis states $\phi_\alpha(r_k)$ with $\alpha = (n,l,s,j,m_j)$
- Radial wavefunctions: Harmonic Oscillator (HO), Woods-Saxon, Coulomb-Sturmian, Complex Scaled HO, Berggren, . . .
- $M$-scheme: Many-Body basis states eigenstates of $\hat{J}_z$
  \[ \hat{J}_z | \Phi_i \rangle = M | \Phi_i \rangle = \sum_{k=1}^{A} m_{ik} | \Phi_i \rangle \]
- $N_{\text{max}}$ truncation: Many-Body basis states satisfy
  \[ \sum_{\alpha \ \text{occ.}}^{A} (2n + l)_\alpha \leq N_0 + N_{\text{max}} \]
  \[ N_{\text{max}} \text{ runs from zero to computational limit.} \]
  \[ (N_{\text{max}}, \hbar \Omega) \text{ fix HO basis} \]
- Alternatives:
  - Full Configuration Interaction (single-particle basis truncation)
  - Importance Truncation
  - No-Core Monte-Carlo Shell Model
  - SU(3) Truncation
  Roth, PRC79, 064324 (2009)
  Abe et al, PRC86, 054301 (2012)
  Dytrych et al, PRL111, 252501 (2013)
Calculation of three-body forces at N^3LO

**Goal**

Calculate matrix elements of 3NF in a partial-wave decomposed form which is suitable for different few- and many-body frameworks.

**Challenge**

Due to the large number of matrix elements, the calculation is extremely expensive.

**Strategy**

Develop an efficient code which allows to treat arbitrary local 3N interactions.

(Krebs and Hebeler)

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Established method for GS energy error estimate adapted to case where results up to N2LO are used:

\[ Q \equiv \frac{m_\pi}{\Lambda} \]

\[ \delta E^{(0)} = \max(Q^2 |E^{(0)}|, |E^{(2)} - E^{(0)}|, |E^{(3)} - E^{(0)}|, |E^{(3)} - E^{(2)}|) \]

\[ \delta E^{(2)} = \max(Q^3 |E^{(0)}|, Q |E^{(2)} - E^{(0)}|, |E^{(3)} - E^{(2)}|, Q \delta E^{(0)}) \]

\[ \delta E^{(3)} = \max(Q^4 |E^{(0)}|, Q^2 |E^{(2)} - E^{(0)}|, Q |E^{(3)} - E^{(2)}|, Q \delta E^{(2)}) \]

Error estimate for finite nuclei results using average relative momentum based on Hartree-Fock results (~NCSM results) at each chiral order:

\[ p_{ij} \equiv \frac{\vec{p}_i - \vec{p}_j}{2} \]

\[ T_{\text{rel}} \equiv \frac{2}{A} \sum_{i<j} \left( p_{ij} \right)^2 \equiv \frac{2}{A} \frac{A(A-1)}{2} \left( p_{\text{avg}} \right)^2 \]

\[ p_{\text{avg}} = \sqrt{\frac{m(T_{\text{rel}})}{A-1}}; \quad Q \equiv \text{Max} \left( \frac{m_\pi}{\Lambda}, \frac{p_{\text{avg}}}{\Lambda} \right) \]

\[ \delta E^{(i)} = Q^{\text{max}(2, i+1)} |V^{(i)}|; \quad \text{where } Q \text{ is evaluated at } i \]
Dimensionless $Q$ based on $p_{\text{avg}}$ from NCSM

$Q = \frac{p_{\text{avg}}}{\Lambda}$ (dimensionless)

$\frac{m_\pi}{\Lambda}$

PRELIMINARY
Note: Black is our new Q with |V|
Green: No “max” condition
Red: Established
Black: New Q with |V|
Blue bands: Extrapolation error
Preliminary light-nuclei results

Ground state energy (MeV)

-80 -70 -60 -50 -40 -30 -20 -10 0

(1/2^+, 1/2) (0^+, 0) (0^+, 2) (1^+, 0) (3/2^-, 1/2) (0^+, 2) (2^+, 1) (3/2^+, 3/2) (0^+, 0) (3/2^-, 1/2)

Experimental data
LO through N^2LO chiral NN potential

\(^{3}\text{H}, ^{4}\text{He}, ^{6}\text{He}, ^{6}\text{Li}, ^{7}\text{Li}, ^{8}\text{He}, ^{8}\text{Li}, ^{8}\text{Be}, ^{9}\text{Li}, ^{9}\text{Be}\)
Ground state energies with $\chi$EFT up to $A = 9$
Next step: Need to apply these analyses to other observables, e.g. $r^2$, $0\nu\beta\beta$, . . .

Now consider truncation vs Okubo-Lee-Suzuki (OLS) renormalization for electromagnetic observables using LENPIC interactions in model problems
Consider two nucleons as a model problem with $V = \text{LENPIC Chiral EFT Interactions (R = 1.0 fm)}$ solved in the harmonic oscillator basis with $\hbar\Omega = 5, 10$ and $20 \text{ MeV}$.

Also, consider the role of an added harmonic oscillator quasipotential

Hamiltonian #1

$$H = T + V$$

Hamiltonian #2

$$H = T + U_{\text{osc}}(\hbar\Omega_{\text{basis}}) + V$$

Evaluate lowest states’ observables:

- Ground state energy $E$
- Root mean square radius $R$
- Magnetic dipole operator $M1$
- Electric dipole operator $E1$
- Electric quadrupole moment $Q$
- Electric quadrupole transition $E2$
- Gamow-Teller $GT$
- Neutrinoless double-beta decay $M(0\nu)$

Dimension of the “full space” is $N_{\text{max}} = 400$ for all results depicted here.
With $H$ defining the OLS transformation, the same picture applies to other Hermitian operators.
"Fractional Difference" is Model-Exact | Exact
PRELIMINARY: Deuteron properties – Truncation vs OLS
Chiral N2LO for Ham #2 (external trap) & LO for other operators

\[ E_{gs} \]

Fractional Difference

\[ R_{rms} \]

Fractional Difference

\[ Q_2 \]

Fractional Difference

\[ \mu_1 \]

Fractional Difference
Consider a 2-body contribution within EFT to $0\nu\beta\beta$-decay at NLO


\[
M^0 = \langle \Psi_{A,Z+2} | \sum_{i,i} \frac{R}{r_{ij}} [F_1(x_{ij})\bar{\sigma}_i\bar{\sigma}_j + F_2(x_{ij})T_{ij}] \tau_i^+ \tau_j^+ | \Psi_{A,Z} \rangle
\]

\[
F_1(x) = (x - 2)e^{-x}, \quad F_2(x) = (x + 1)e^{-x}, \quad x = m_\pi |\vec{r}|
\]

\[
T_{ij} = 3\bar{\sigma}_i\hat{r}_{ij}\bar{\sigma}_j\hat{r}_{ij} - \bar{\sigma}_i\bar{\sigma}_j
\]

Additional operators being developed – stay tuned

Regulator applied to operators for consistency when using LENPIC interactions

\[
f \left( \frac{r}{R} \right) = \left( 1 - \exp \left( -\frac{r^2}{R^2} \right) \right)^6
\]

\[R = 0.8, \ 0.9, \ 1.0, \ 1.1, \ 1.2 \ \text{fm} \]
0vββ for 1S0(nn) → 1S0(pp) using Ham #2 (external trap)
Roles of chiral order, consistent regularization and OLS renormalization
Plans:

Implement in finite nuclei:

Input OLS’d operators as TBMEs in single-particle representation

Perform benchmark $A=6$ calculations with UNC group (underway)

Evaluate/save density matrices (static and transition) and use them to evaluate OLS’d observables and compare with results from bare observables

Expand treatment to wider range of EW operators within Chiral EFT at NLO & N2LO

Extend to 3-body H with OLS on operators at the 3-body level

Extend to medium weight nuclei with “Double OLS” approach
Double OLS reduction of the basis to a “conventional” shell model valence space

\[ N'_{\text{max}} = 0 \]

\[ P'H'_{\text{eff}}P' \]

\[ P'H_{\text{eff}}P = 0 \]

\[ QH_{\text{eff}}P = 0 \]

\[ QH_{\text{eff}}Q = 0 \]

Dikmen, Lisetskiy, Barrett, Maris, Shirokov, Vary, PRC 91, 064301 (2015); arXiv 1502:00700
Collaborators at Iowa State University and NUCLEI Team members

Robert Basili (grad student)
Weijie Du (grad student)
Matthew Lockner (grad student)
Pieter Maris
Soham Pal (grad student)
Shiplu Sarker (grad student)

Note: Proposed faculty hire at Iowa State in NP with support from the Fundamental Interactions Topical Collaboration
Conclusions

Uncertainty vs chiral order is consistent when adopting avg relative momentum from NCSM to set the dimensionless scale $Q$ along with $|V|$ for the energy scale.

OLS succeeds in renormalizing the IR and UV scales in these initial applications to electroweak operators.

Outlook

Novel approach to scattering now established and used to predict the tetraneutron. Opens a path for scattering applications with chiral interactions in light nuclei.

Major additional efforts needed to develop and apply these methods: effective Hamiltonians, effective electroweak operators, many-body methods, . . . .