Regulators and Revisiting the DME

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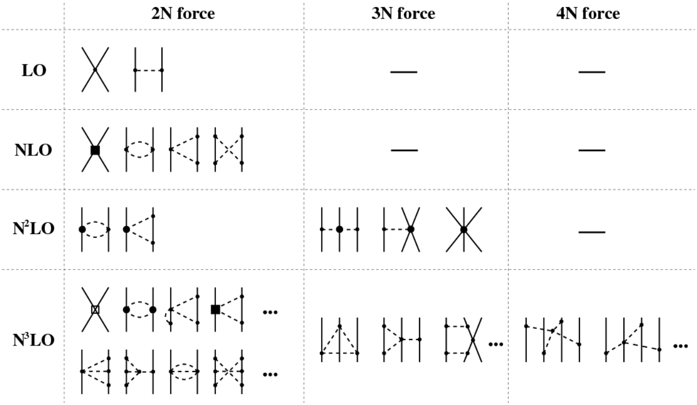
U.S. DEPARTMENT OF ENERGY

NSF

THE OHIO STATE UNIVERSITY

NUCLEI
Nuclear Computational Low-Energy Initiative

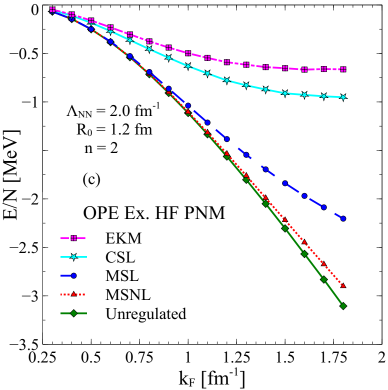
χEFT Introduction



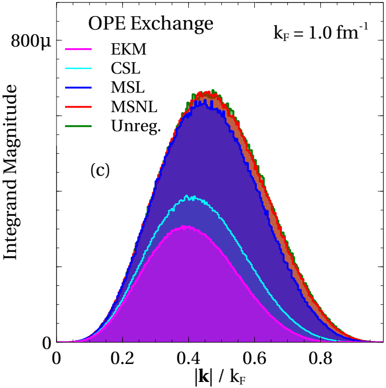
- Effective field theory utilizing relevant d.o.f. (nucleons, pions) for low-energy nuclear physics
- In the precision era, ab initio results provides benchmarking
- Caveat: expansion is non-renormalizable order by order $\Longrightarrow$ pay attention to regulators and cutoffs!

Regulator Results in Uniform Matter

OPE Exchange Fock energy



OPE Fock integrand



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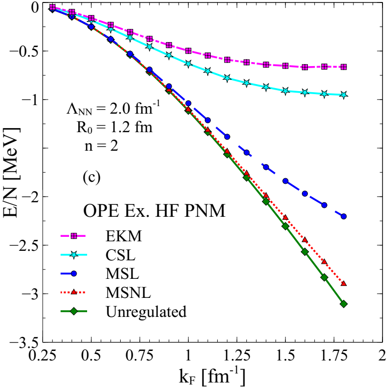

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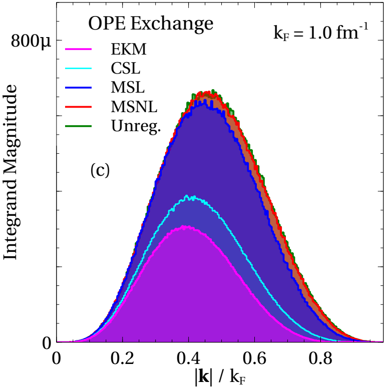
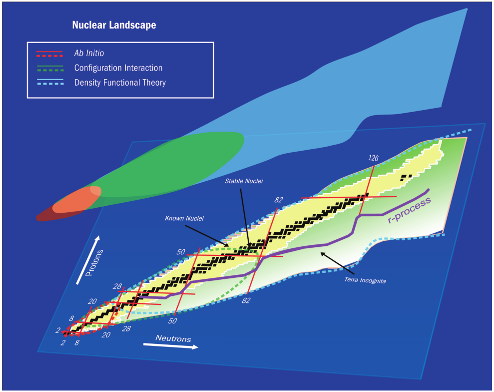


Takeaway:

- Regulators can significantly affect results (for much more see arxiv:1602.08038)
- Motivation for revisiting DME using regulators!

Intro to Nuclear EDF

- DFT methods are the only reliable way to calculate all nuclei
- Basic object is the energy functional $E[\rho]$
- **Question**: Does adding pion physics improve existing Skyrme functionals?



Bottom Line

Seeking model independent predictions across the nuclear chart

Energy Functional 101

Variables are different local densities and their derivatives

$$E[\rho] = \int \mathcal{H}(\mathbf{r}) d\mathbf{r}$$

$$\mathcal{H}(\mathbf{r}) = \frac{\hbar^2}{2m}\tau_0 + \sum_{t=0,1} C_t^{\rho\rho}\rho_t^2 + C_t^{\rho\tau}\rho_t\tau_t + C_t^{\rho\Delta\rho}\rho_t\Delta\rho_t + \dots$$

Dictionary

- $\rho_t(\mathbf{r})$ - local density at $\mathbf{r}$
- $\tau_t(\mathbf{r})$ - kinetic energy density at $\mathbf{r}$
- C_t are couplings (fit to nuclear data for Skyrme)
- Terms come in isoscalar ($t = 0$) and isovector ($t = 1$) flavors

Overview

Plan

- Start with a Skyrme-like functional (empirical) then include pion physics via chiral potentials
- Pion physics gives non-empirical density-dependent couplings, refit contact couplings to data
- Long-range in-medium interaction resembles vacuum interaction

Goals

- Reproduce success of Skyrme phenomenology (first do no harm)
- Go beyond Skryme "1 MeV wall"
- Look for systematic improvement order by order in the chiral expansion

Signs of Success

1. **Global**: Decrease in χ^2 for fit to all nuclei
2. **Local**: Look for systematic improvement across isotope chains

Adding Pions: HF in DFT Language

Express HF energy in terms of 1-body density matrices (1BDM) $\rho(\mathbf{x}_1, \mathbf{x}_2)$

$$V_{\mathrm{HF}} = \frac{1}{2} \sum_{i,j}^{A} \langle ij|\mathcal{V}|ij\rangle \;, \qquad \mathcal{V} \equiv V(1 - P_{12})$$

$$V_{\mathrm{HF}} = \frac{1}{2} \int \prod_{i=1}^{4} d\mathbf{r}_i \; \langle \mathbf{r}_1\mathbf{r}_2|\mathcal{V}|\mathbf{r}_3\mathbf{r}_4\rangle \; \rho(\mathbf{r}_3, \mathbf{r}_1) \; \rho(\mathbf{r}_4, \mathbf{r}_2)$$

$$\rho(\mathbf{r}_1, \mathbf{r}_2) \equiv \sum_{i}^{A} \phi_i^*(\mathbf{r}_2)\phi_i(\mathbf{r}_1) \;, \quad \rho(\mathbf{r}, \mathbf{r}) = \rho(\mathbf{r})$$

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After converting to CMS coordinates and performing an integral,

$$\begin{aligned} V_{\mathrm{HF}} = {} & \frac{1}{2}\int d\mathbf{R}d\mathbf{r}\ V(\mathbf{r})\ \rho(\mathbf{R}+\mathbf{r}/2,\mathbf{R}+\mathbf{r}/2)\ \rho(\mathbf{R}-\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2) \\ & -\frac{1}{2}\int d\mathbf{R}d\mathbf{r}\ V(\mathbf{r})\ \rho(\mathbf{R}+\mathbf{r}/2,\mathbf{R}-\mathbf{r}/2)\ \rho(\mathbf{R}-\mathbf{r}/2,\mathbf{R}+\mathbf{r}/2) \end{aligned}$$

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Exchange term's 1BDM is not diagonal $\implies$ nonlocal Fock term

Building Local Functionals

Density Matrix Expansion (DME) Basics

- Way to map nonlocal functionals into local ones
- Decompose 1BDM into (iso)scalar/(iso)vector terms
- Expand decomposed 1BDMs about the diagonal, e.g.,

$$\rho_t(\mathbf{R} + \mathbf{r}/2, \mathbf{R} - \mathbf{r}/2) \approx \sum_{n=0}^{n_{\max}} \Pi_n(kr)\mathcal{P}_n(\mathbf{R})$$

$$k \equiv \text{momentum scale}\;, \qquad \mathcal{P}(\mathbf{R}) \in \{\rho(\mathbf{R}), \tau(\mathbf{R}), \ldots\}$$

- Exchange term now approximated by density-dependent couplings (Π functions) and products of local densities ($\mathcal{P}(\mathbf{R})$ terms)
- Previous formulation done in momentum space, no regulators, with improvements over Negele-Vautherin

Gebremariam et al. Nucl. Phys. A 851 (2011)

Coordinate Space DME

Coordinate Space Advantages

1. Explicitly separates out short-range parts of the long-range terms (e.g., OPE delta function)
2. Allows use of coordinate space regulators
3. Changing regulator cutoff $\Longrightarrow$ adiabatically turn on the pion terms (functional coefficients should evolve continuously)

Challenge: Including 3N Forces

Standard Way

- 3N Forces difficult to handle via standard DME formalism
- Traces over 3-body spin-isospin are monstrous

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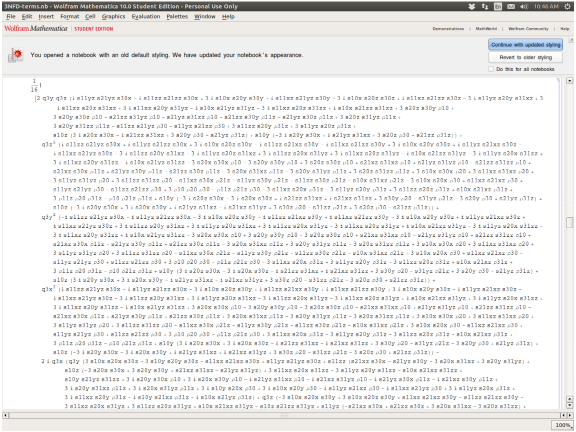
E.g., one part of the V_D (3N OPE) spin-isospin traces



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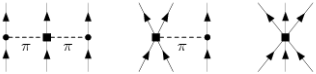
Standard Way

- 3N Forces difficult to handle via standard DME formalism
- Traces over 3-body spin-isospin are monstrous
- Traces only first step, still need to expand 1BDMs ...

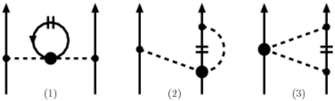
Alternative Procedure - Averaged 3N

- Average one leg of the 3-body force $\Longrightarrow$ effective 2-body forces



c_1, c_3, c_4 c_D c_E

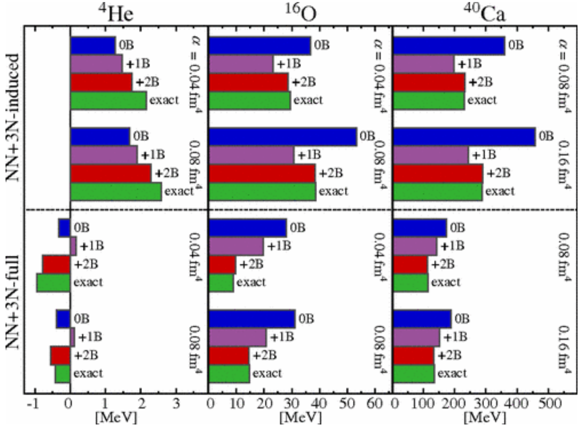
$\Longrightarrow$



- Averaging initially done in momentum space (e.g., applied in coupled cluster), proceed in coordinate space for similar reasons as above

Efficacy of Effective 2-Body Forces

- Ab initio results suggest residual 3-body terms are mostly negligible



Roth et al. PRL 109 (2012)

- $\langle V^{3N} \rangle$ and normal ordered components in light nuclei

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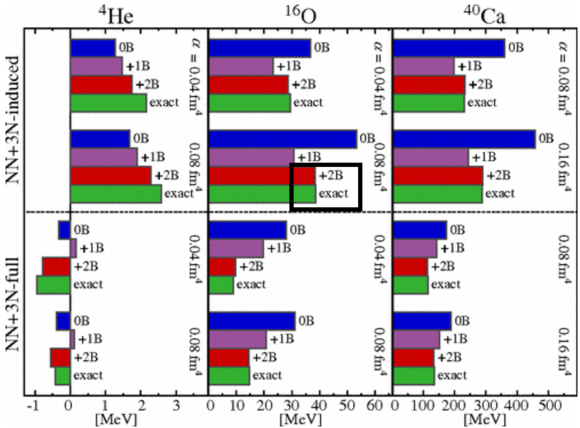
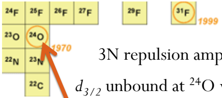


Roth et al. PRL 109 (2012)

- $\langle V^{3N} \rangle$ and normal ordered components in light nuclei
- Including up to 2-body terms well approximates exact result

Evidence for 3N Forces

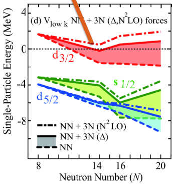
In microscopic shell model, dripline at ^{24}O understood by repulsive 3N forces pushing up $d_{3/2}$ state.

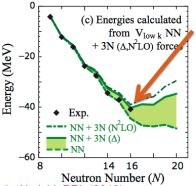


Probe limits of nuclear existence with 3N forces

3N repulsion amplified with N: ***vital for neutron-rich nuclei***

$d_{3/2}$ unbound at ^{24}O with 3N forces





Otsuka, Suzuki, Holt, Schwenk, Akaishi, PRL (2010)

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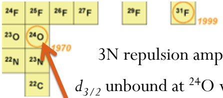

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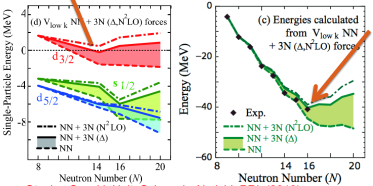

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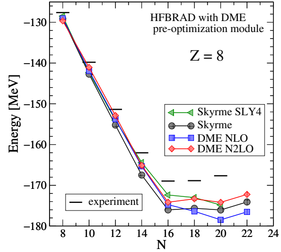
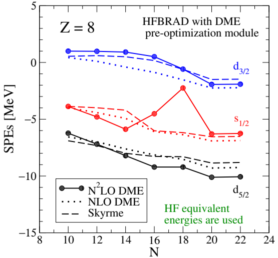


Stoitsov et al. PRC 82 (2010)



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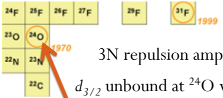

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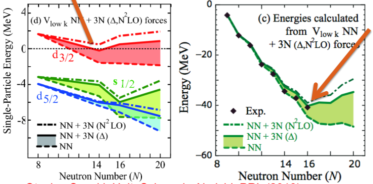

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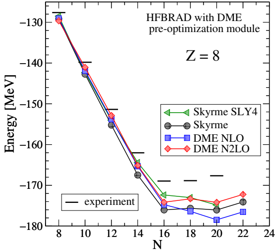

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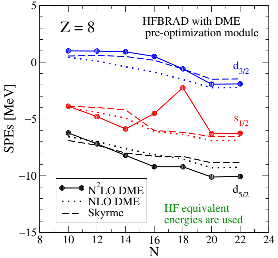

Dripline at ^{24}O but no change in $d_{3/2}$ state...
Stay tuned!

Other Candidates

- systematics (e.g. radii) in the calcium chain
- kink in charge radius for the lead chain

Summary and Outlook

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1. Regulators can have an impact on nuclear observables in χEFT

   A. Dyhdalo et al., "Regulator Artifacts in Uniform Matter for Chiral Interactions", arXiv:1602.08038 (to be published in PRC)

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Future Work

1. Test new local functional with coordinate space chiral potentials, regulators, and 3N forces (with MSU and LLNL)
2. Include pairing and move towards ab initio functionals
3. Explore alternative regulators and artifacts from Fierz ambiguity