

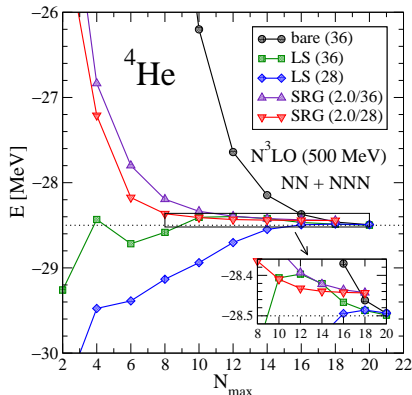
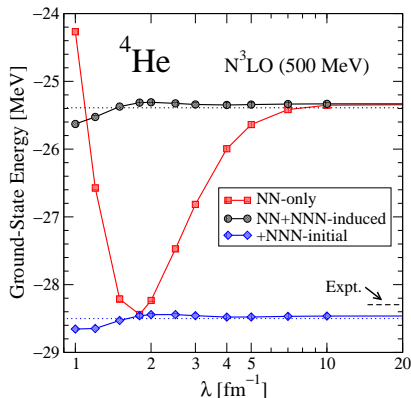
Role and Goals of the Ab Initio Functionals Group

- 1 Provide interactions for ab initio structure methods
 - low-momentum interactions ($V_{\text{low } k}$, SRG)
 - advantageous convergence for some methods
 - driven by requirements of ab initio DFT
 - multiple resolutions: cut-off dependence as a diagnostic
 - 3NF is essential ingredient
 - evolved consistently with NN or fit to chiral EFT basis
 - alternatives: density dependent NN, in-medium SRG
- 2 Develop novel density dependencies for EDF's based on microscopic interactions
 - universal long-range chiral EFT
 - input to and interaction with DFT applications group
- 3 Develop complete ab initio (from NN...N) DFT
 - test approximations against ab initio (and experiment!)
 - use external fields and Hamiltonian parameters to probe
 - understand conceptual issues (e.g., symmetry breaking)

Interaction (so far) with CS/AM and HPC primarily through
Ab Initio Structure and DFT Applications groups.

Year 3 Highlights from Graduate Students

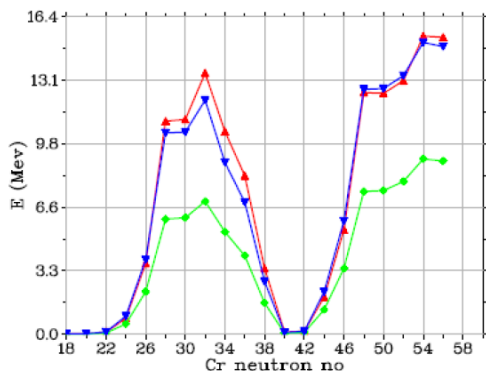
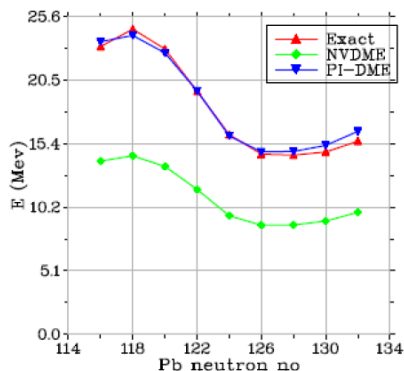
- Eric Jurgenson: Consistent SRG evolution of 3NF



- “Evolution of nuclear many-body forces with the similarity renormalization group,” E.D. Jurgenson, P. Navratil and R.J. Furnstahl, arXiv:0905.1873
- HO matrix elements \implies ab initio structure

Year 3 Highlights from Graduate Students

- Biruk Gebremariam: Phase-space-averaging extensions of Negele-Vautherin (NV) density matrix expansion (DME)



- Also Biruk: Analytic DME for long-range chiral EFT (3NF!) calculated and delivered to DFT Applications group
- Many papers (with S. Bogner, T. Duguet) in progress!

Year 3 Accomplishments (Deliverables)

- NN ··· N interactions \implies 3NF
 - new 3NF: additional $V_{\text{low } k}$ /SRG fits, SRG-evolved 3NF
 - progress toward density-dependent NN for 3NF (TRIUMF)
 - first in-medium SRG calculations (infinite matter, light nuclei)
- Completed low- k (momentum-space, 3NF) scalar NV-DME
 - “Density matrix expansion for low-momentum interactions,” S.K. Bogner, R.J. Furnstahl, and L. Platter, Eur. Phys. J. **A39**, 219 (2009)
 - identified limitations of scalar NV-DME based on HFBRAD-implementation and CC comparisons
- Completed DME for long-range chiral EFT NN and 3NF
 - *all* analytic expressions from fully automated tools
 - codes delivered (and freely available)
- Completed improved DME for vector part (PSA Π -DME)
 - parameter free; greatly reduced errors from NV-DME
- Further development of non-empirical pairing using $V_{\text{low } k}$
- First steps toward orbital-based DFT (1D models)
 - “Toward ab initio density functional theory for nuclei,” J.E. Drut, R.J. Furnstahl, and L. Platter, arXiv:0906.1463 [nucl-th]

Articles and Preprints Citing SCIDAC Support

- ✓ Published or Posted since Pack Forest 2008
 - “Decoupling in the similarity renormalization group for nucleon-nucleon forces,” E.D. Jurgenson, S.K. Bogner, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **78**, 014003 (2008)
 - “Density matrix expansion for low-momentum interactions,” S.K. Bogner, R.J. Furnstahl, and L. Platter, Eur. Phys. J. **A39**, 219 (2009)
 - “Similarity renormalization group evolution of many-body forces in a one-dimensional model,” E.D. Jurgenson and R.J. Furnstahl, Nucl. Phys. A **818**, 152 (2009)
 - “Nuclear matter from chiral low-momentum interactions,” S.K. Bogner, R.J. Furnstahl, A. Nogga and A. Schwenk, arXiv:0903.3366 [nucl-th], submitted to PRL
 - “Evolution of nuclear many-body forces with the similarity renormalization group,” E.D. Jurgenson, P. Navratil and R.J. Furnstahl, arXiv:0905.1873, submitted to PRL
 - “Toward ab initio density functional theory for nuclei,” J.E. Drut, R.J. Furnstahl, and L. Platter, arXiv:0906.1463 [nucl-th], commissioned review for Prog. Part. Nucl. Sci.



Many papers soon from MSU/Saclay collaboration!

Plans for Rest of Year 3 and Year 4 and ...

Plans are nothing; planning is everything. — Dwight D. Eisenhower

- 3NF fits and tests
 - 3NF project to interface $V_{\text{low } k}$ chiral EFT 3NF with NCFC
 - Test new fits with CC and NCFC in larger nuclei (e.g., λ/Λ dependence)
 - Use NCFC in light nuclei for fits of N²LO 3NF coefficients C_D , C_E (and c_i 's) for many SRG and smooth $V_{\text{low } k}$ cutoffs
- Evolving 3NF with SRG
 - Harmonic oscillator matrix elements for input to NCFCs, CC
 - Understand 3D many-body power counting and use to estimate higher-body interactions; evolve operators
 - Momentum-space evolution of 3NF
 - Validate 3NF chiral basis fits vs. evolved 3NF
- Develop and test in-medium SRG
 - Uniform systems, light closed-shell nuclei
 - Shell model effective interaction
- Upgrade SRG input as it develops (N³LO 3NF, Δ 's, ...)
 - Relies on outside people

Plans for Rest of Year 3 and Year 4 and ...

- Nuclear matter calculational extensions
 - Full 2nd order calculation with fit 3NF (w/TRIUMF)
 - Asymmetric nuclear matter (just coding to finish)
 - Solve uniform matter with in-medium SRG
 - Explore coupled cluster for nuclear matter (UT/ORNL)
- Nuclear matter studies
 - Complete and publish the G-matrix and BBG study
⇒ test power counting with numerical examples
 - Nonperturbativeness in the particle-hole channel
 - Pairing, e.g., in 3S_1
 - Nuclear/neutron matter with Jisp-16 (MSU/ISU)
 - 4NF from N^3LO chiral EFT at Hartree-Fock
- Validating (or invalidating) NV DME from $V_{low k}/SRG$
 - Compare energies, ρ 's to CC, NCFC with same Hamiltonian
 - Vary contact 3NF strength, full 3NF-fitted $V_{low k}/SRG$
 - Compare in external potentials with NCFC, GFMC/AFMC
 - neutron drops

Plans for Rest of Year 3 and Year 4 and ...

- Further development of Π -DME (MSU, Saclay/Lyon)
 - Finish phase space averaging; alternatives for local k_F
 - Write up papers!
 - Validate against exact Hartree-Fock
 - Extend DME to pairing
 - DME beyond HF level — dispersive effects using short-time/factorization methods
- Refit “Skyrme + long-range DME” studies (w/ORNL)
 - Incorporate in HFB DME codes; refit generalized Skyrme
 - Naturalness constraints, higher gradients, look for pion, ...
 - “Non-empirical” DFT with gradients and volume density dependencies constrained from long-range DME
- Continue 1D (3D) development of orbital-based DFT
 - KLI approximations vs. full OEP
 - Model tests against DME; full comparison
 - Issues: self-interaction, self-pairing, ...
 - Symmetry breaking, long-range correlations ...