UNEDF SciDAC Collaboration

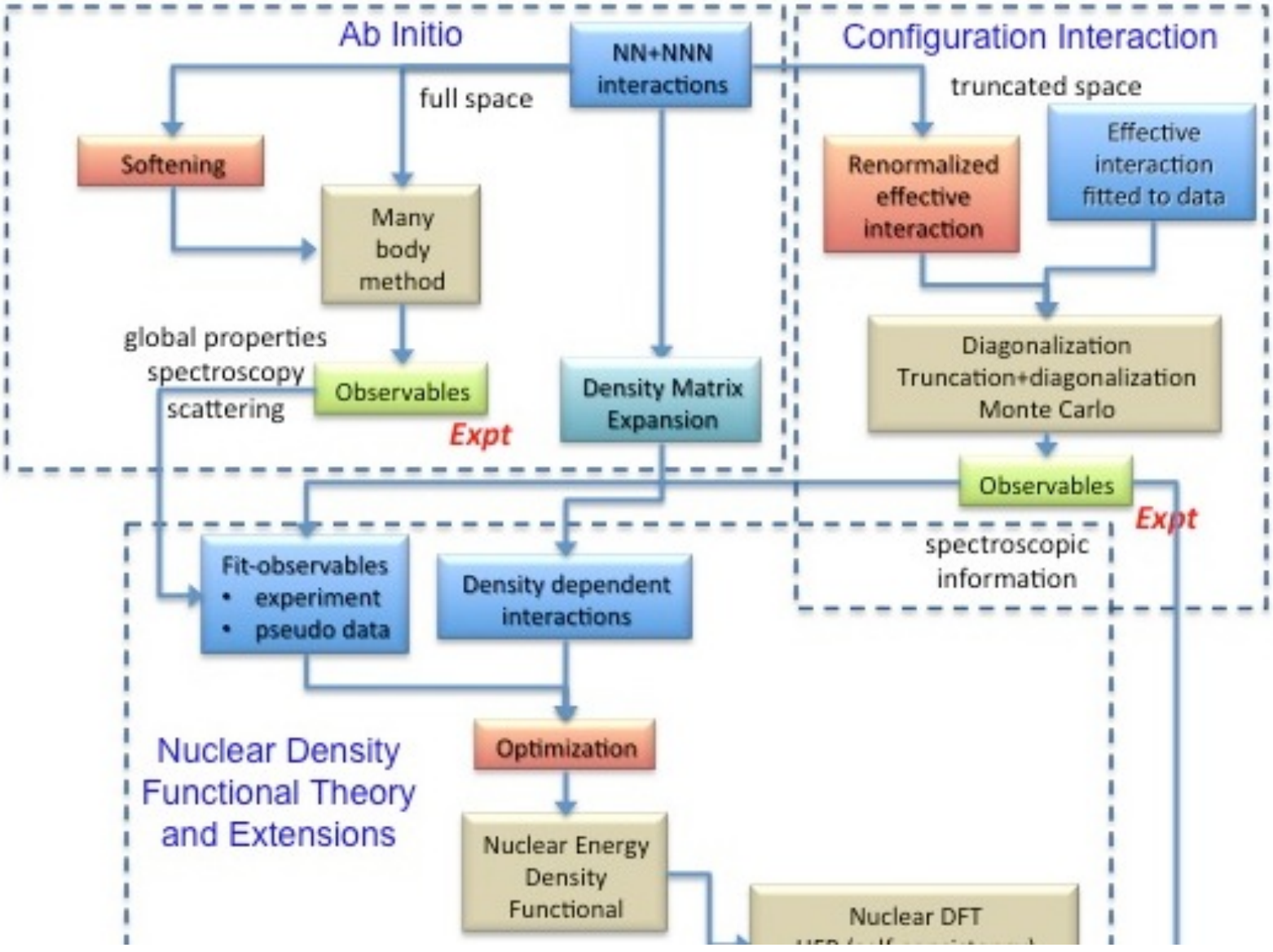
Universal Nuclear Energy Density Functional

Ab Initio Functionals Summary Report

Dick Furnstahl

Department of Physics
Ohio State University

June, 2011


Ab Initio
NN+NNN interactions
full space
Softening
Many body method
global properties
spectroscopy
scattering
Observables
Expt
Density Matrix Expansion
Configuration Interaction
truncated space
Renormalized effective interaction
Effective interaction fitted to data
Diagonalization
Truncation+diagonalization
Monte Carlo
Observables
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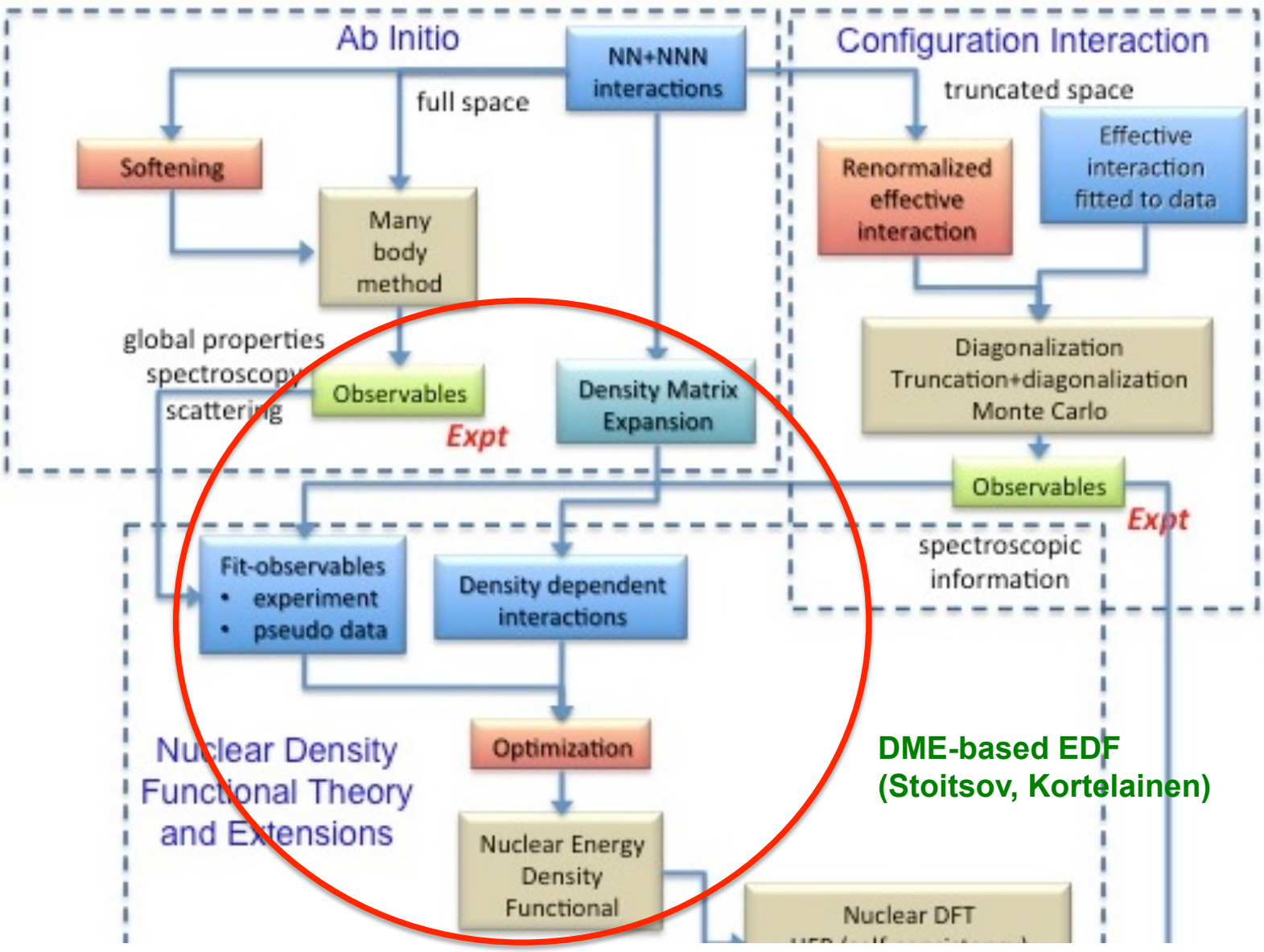
spectroscopic information
Fit-observables
• experiment
• pseudo data
Density dependent interactions
Optimization
Nuclear Density Functional Theory and Extensions
Nuclear Energy Density Functional
Nuclear DFT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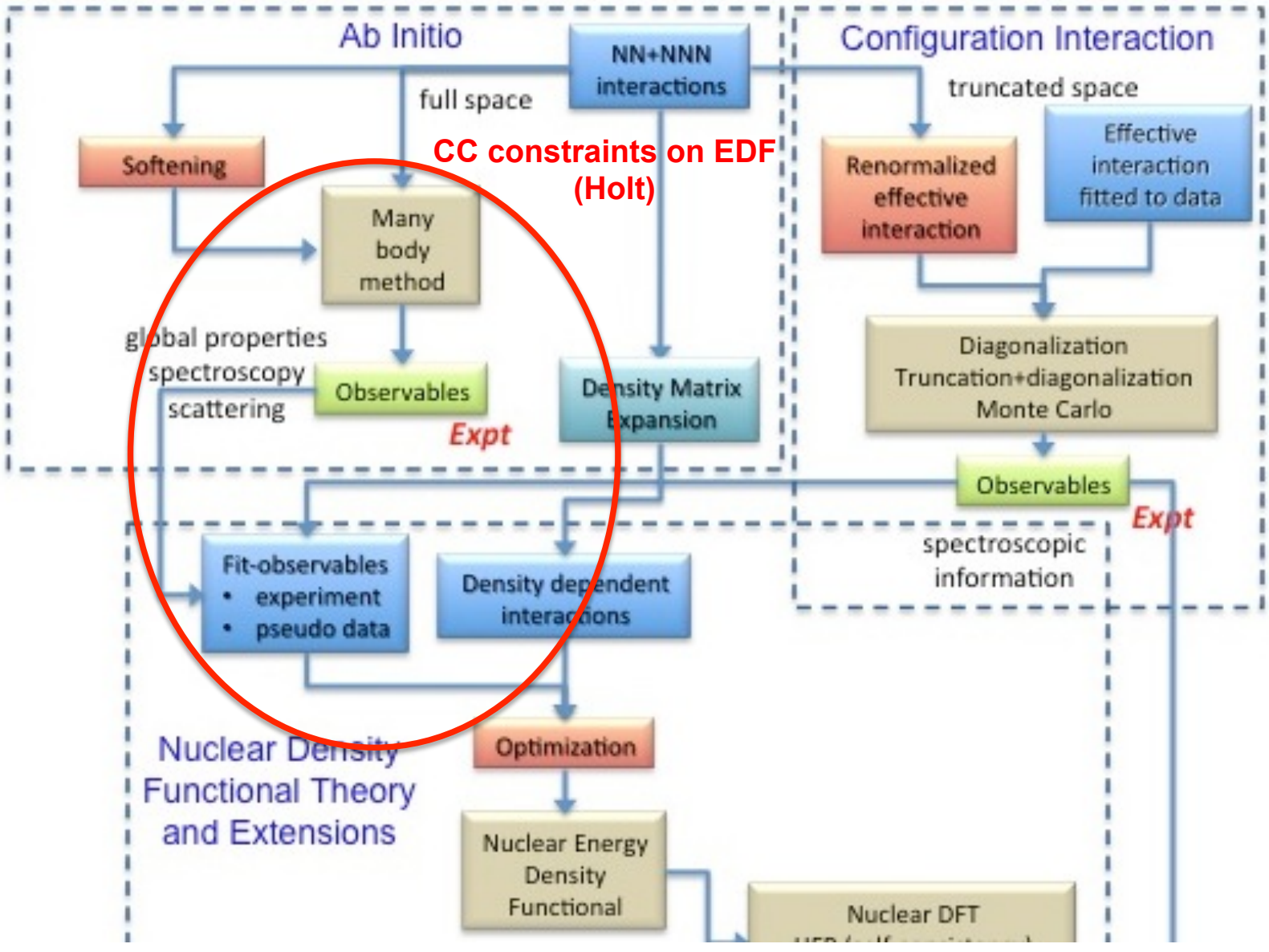
DME-based EDF
(Stoitsov, Kortelainen)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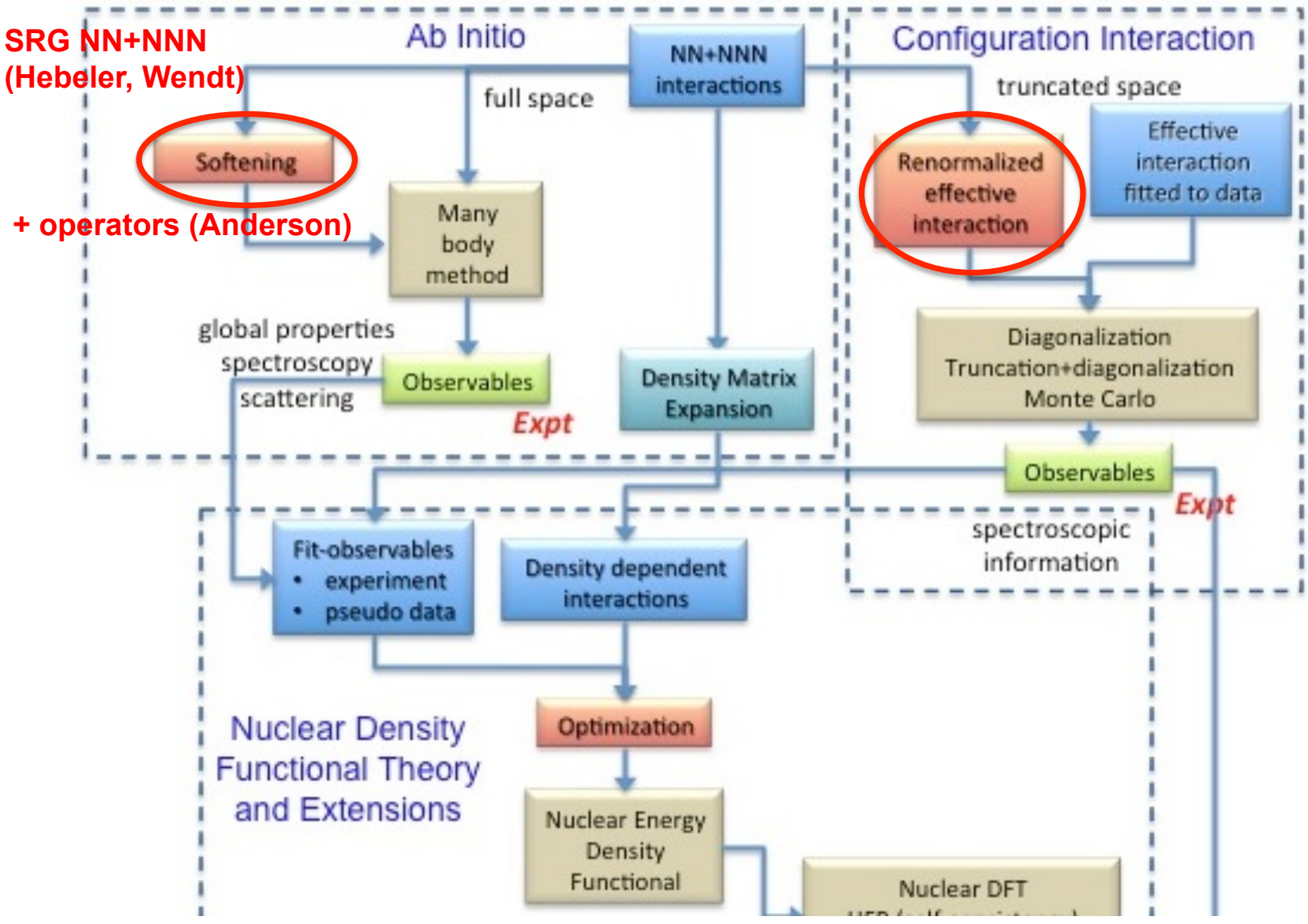
SRG NN+NNN
(Hebeler, Wendt)
+ operators (Anderson)
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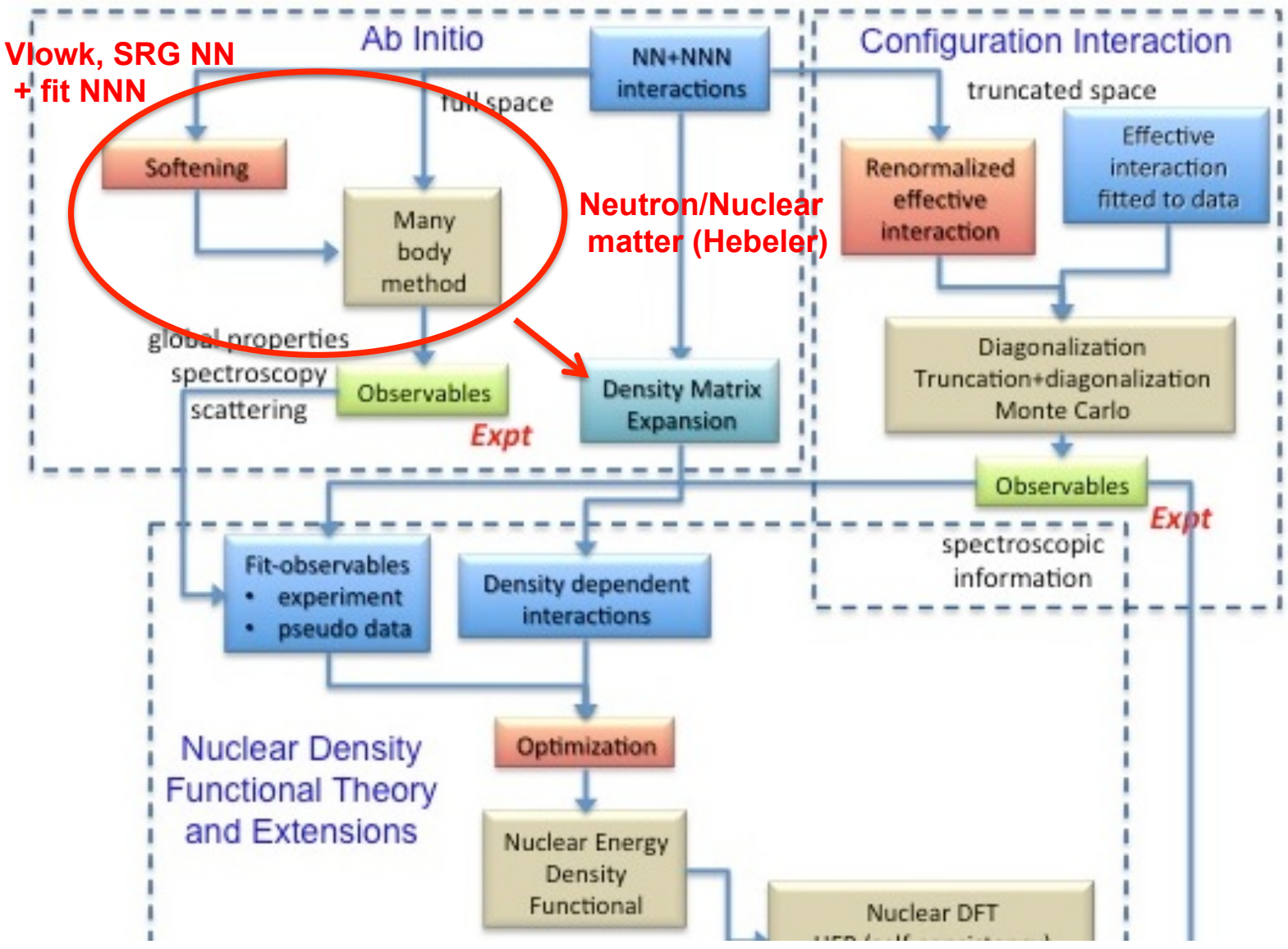
Vlowk, SRG NN
+ fit NNN
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matter (Hebeler)
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Functional Theory
and Extensions
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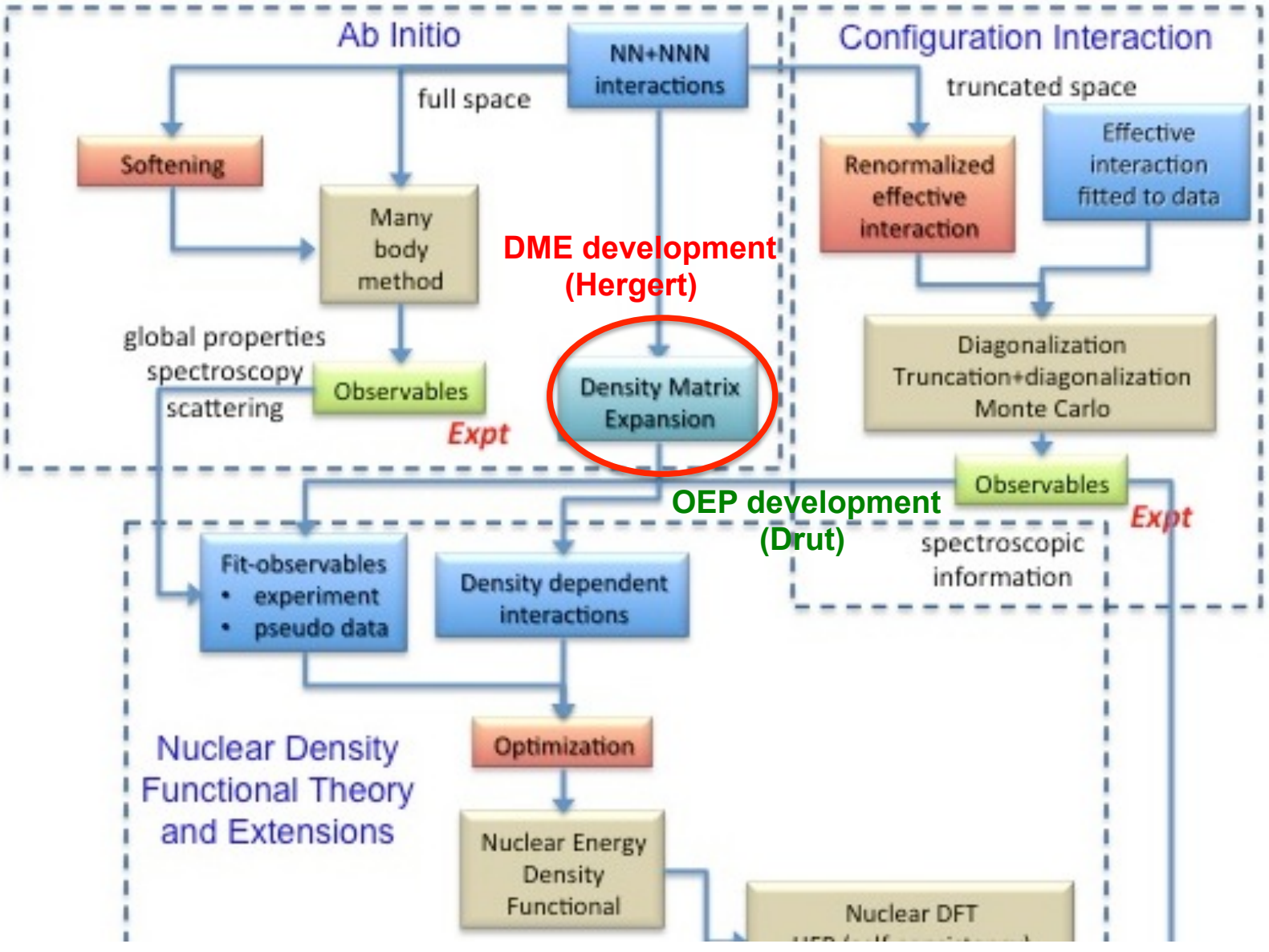
Density
Functional
Nuclear DFT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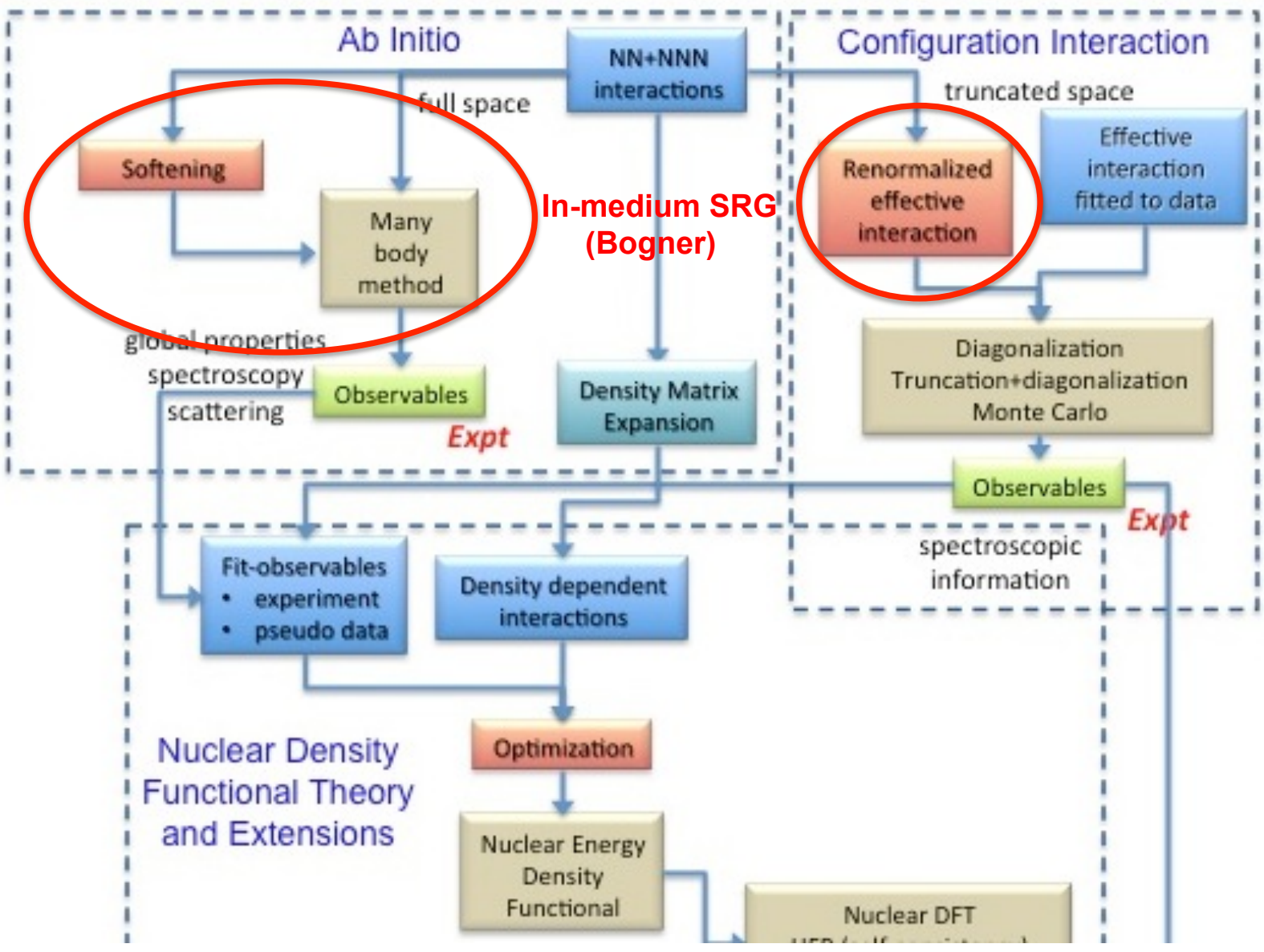
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Ab Initio Nuclear DFT Deliverables

Plan for Year-5 from Continuation Progress Report

- Develop and test improved DME functionals that go beyond HF (microscopic pairing; constrain volume terms from BHF).
- Perform neutron drop benchmarks starting from NN and NNN interactions and validate against ab-initio calculations.
- Develop the Optimized Effective Potential (OEP) method for 3D-HFB; compare with HF, HF-DME, and ab initio.
- Use in-medium SRG to develop valence shell model Hamiltonians and effective operators for open-shell nuclei.

Other deliverables from CPR

- Compare DME to CC and NCFC with the same (variable) Hamiltonian, including with external fields.
- Improve and test infinite matter on which DME relies; initial steps toward Monte Carlo and CC calculations
- Apply $NN + NNN$ low-k SRG interactions in p-shell with NCFC
- SRG: develop few-body operators, test factorization, explore alternative generators to control many-body operators

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Testing the density matrix expansion against ab initio calculations of trapped neutron drops

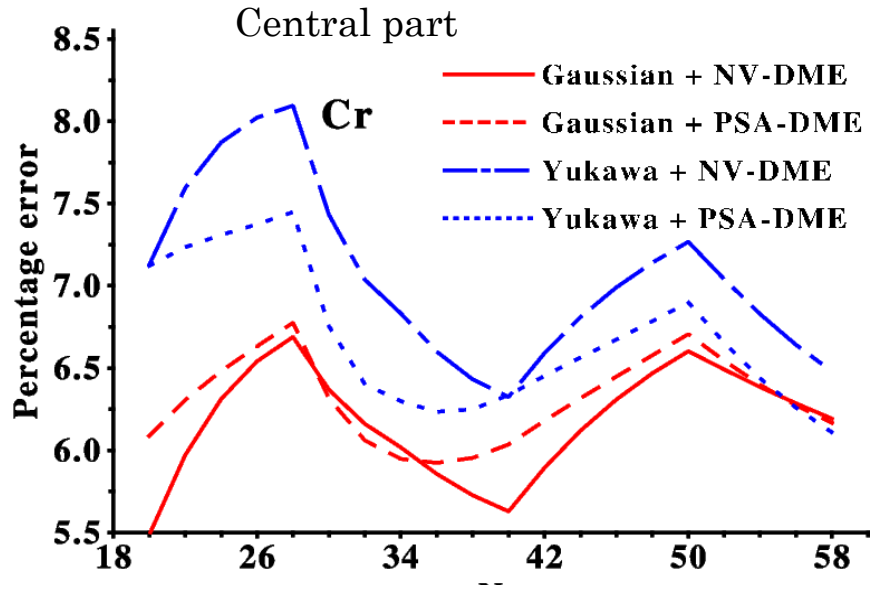
S.K. Bogner, R.J. Furnstahl, H. Hergert,
MK, P. Maris, M. Stoitsov, and J.P. Vary,
arXiv:1106.3557 [nucl-th]

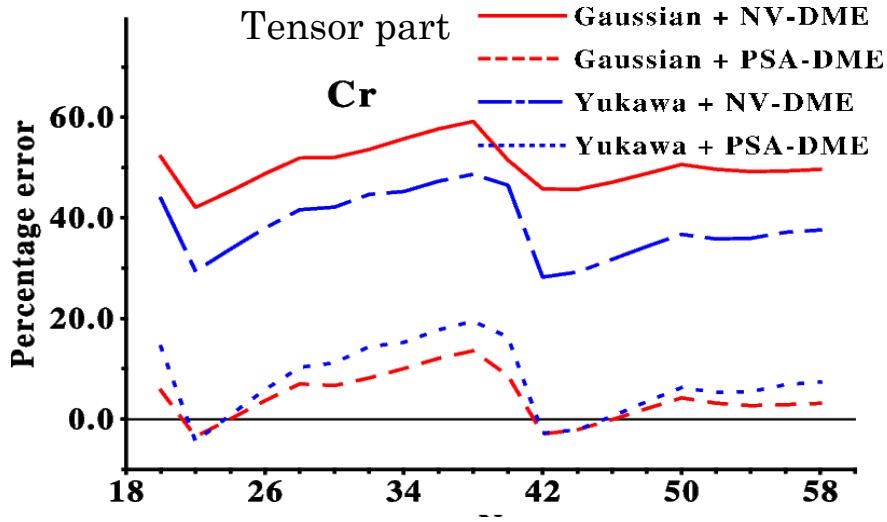
Density matrix expansion

- we have used Negele-Vautherin (NV) and phase-space averaging (PSA) DME
- in DME nonlocal density matrix is expanded to sums of local densities $\mathcal{P}_n(\boldsymbol{R})$

$$\rho_t(\boldsymbol{r}_1, \boldsymbol{r}_2) \approx \sum_{n=0}^{n_{\max}} \Pi_n(kr)\ \mathcal{P}_n(\boldsymbol{R})$$

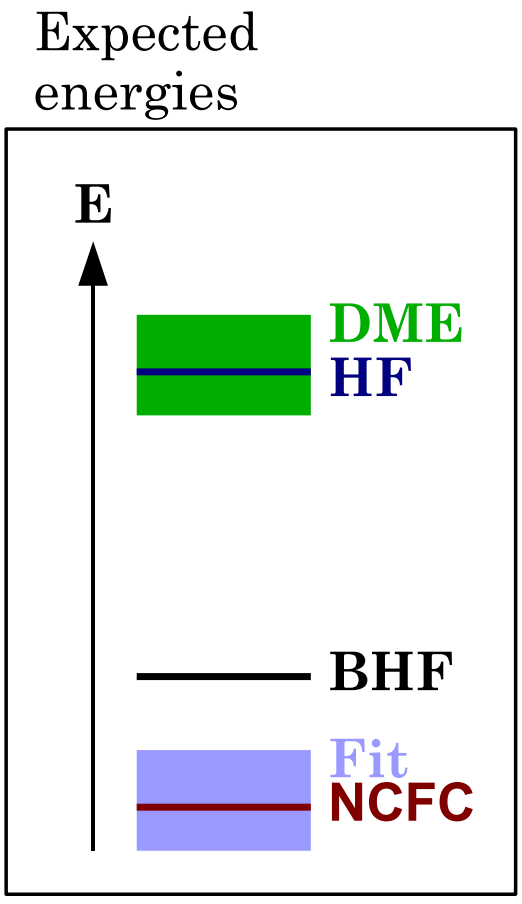
- Π-functions depend on the chosen DME
- for PSA see B. Gebremariam, T. Duguet, and S. K. Bogner, PRC82, 014305 (2010) and S. Bogner's talk on last year's UNEDF meeting
- DME expressions in HFB solvers handled with similar module as in χ-DME EDF case





From PRC82, 014305 (2010)

Comparison of different many body methods



- Minnesota potential (NPA286, 53 (1977)) provides a simple and nontrivial test case for DME
- N=8 and N=20 systems considered
- exact MB results from NCFC calculations
- NV and PSA DME applied to potential to produce semi-local EDF. Results from this EDF can be compared exact HF calculation
- Additional correlations introduced from BHF calculations on infinite neutron matter (INM)
- the ratio of HF and BHF results in INM is a smooth function of density, $f(k_F)$ → scale the DME functional with $f(k_F)$. This is denoted as BHF
- second option is to include BFH correlations by adding contact part to the EDF. Volume part was fitted to BHF INM and surface coupling constant to NCFC total energies. This is denoted as Fit.
- BHF and Fit expected to be close to NCFC results

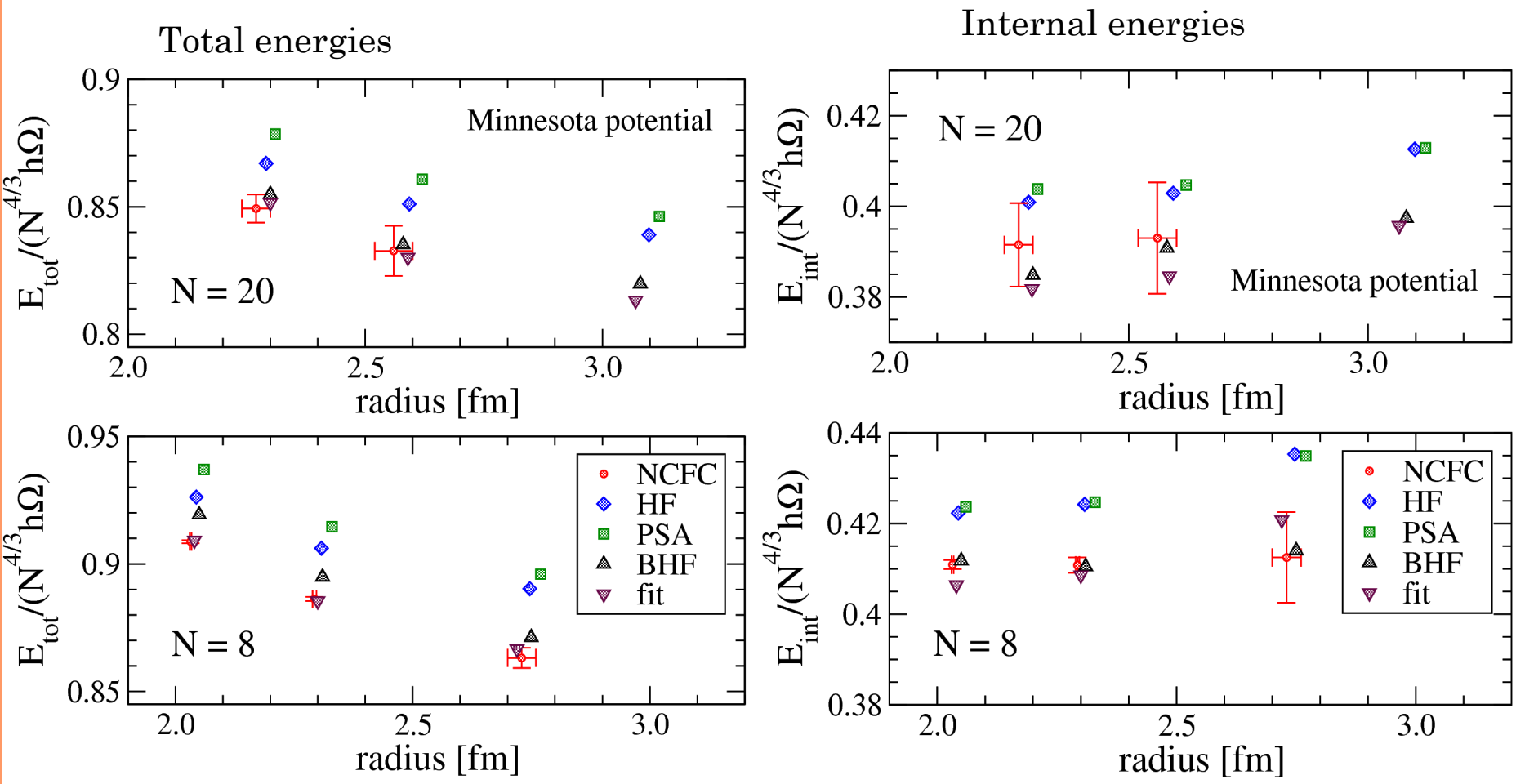
Comparison of NV and PSA DME to HF

- DME can be applied to the Fock term, or on both Hartree and Fock terms
- PSA with exact treatment of Hartree term provides closest results to exact HF
- DME energies calculated from exact HF densities are almost identical to self consistent DME energies

Difference in total energy compared to exact HF in MeV

		HF/NV			HF/PSA		
N	$\hbar\Omega$	NV	NT	exact	PSA	NT	exact
8	3	0.1	0.2	0.1	0.0	0.1	0.0
8	5	0.4	0.8	0.4	−0.1	0.6	0.2
8	10	2.1	5.1	2.0	−1.7	4.1	0.9
8	15	4.2	12.9	4.6	−7.1	10.8	2.1
8	20	6.0	24.2	7.7		20.9	3.4
20	3	0.5	0.8	0.6	−0.1	0.4	0.2
20	5	1.8	3.4	2.3	−1.0	2.0	0.9
20	10	5.9	18.5	11.0	−14.0	12.0	3.9
20	15	3.8	44.3	22.7		31.6	7.9
20	20	−17.8	80.0	34.8		61.3	12.5

DFT and NCFC results compared



$\hbar\omega$ = 20,15,10 MeV (from left to right in figures)

Some Conclusions

- neutron droplets provide a controllable environment to test different many-body methods
- PSA with exact treatment of Hartree term closest to exact HF results
- BHF results closer to NCFC results than bare DMA results, but still outside of the theoretical error bars
- Fit results often inside of the theoretical error bars, but not always. Generally they have good agreement
- year 5 deliverables: neutron drop calculations from NN interaction validated against ab-initio calculations
- next step: test χ-DME EDF against exact HF and ab-initio calculations, include pairing

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Phenomenological N^{3}LO functionals for nuclei

Jacek Dobaczewski
University of Warsaw & University of Jyväskylä

In collaboration with the FiDiPro team:
Gillis Carlsson, Nicolas Michel, Alessandro Pastore,
Francesco Raimondi, Jussi Toivanen, Pekka Toivanen, Petr Veselý

UNEDF Annual Collaboration Meeting
June 20-24, 2011, Michigan State University

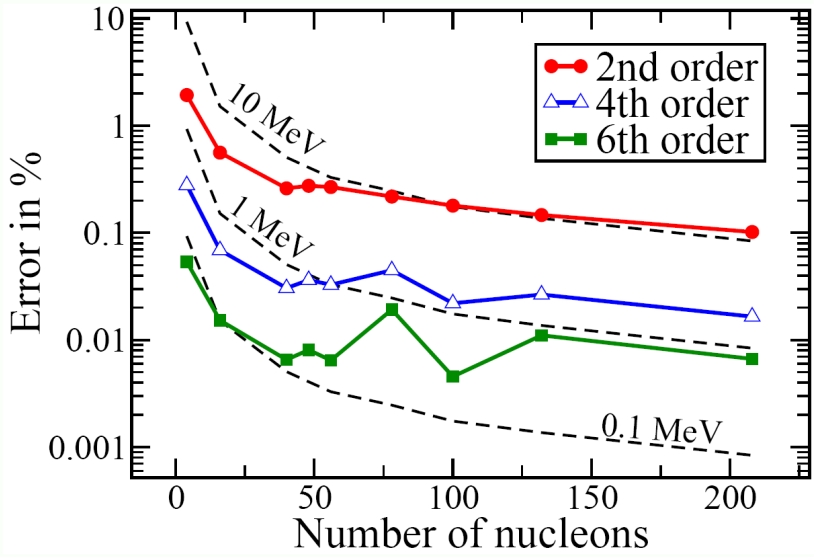
JYVÄSKYLÄN YLIOPISTO

Convergence of the DME

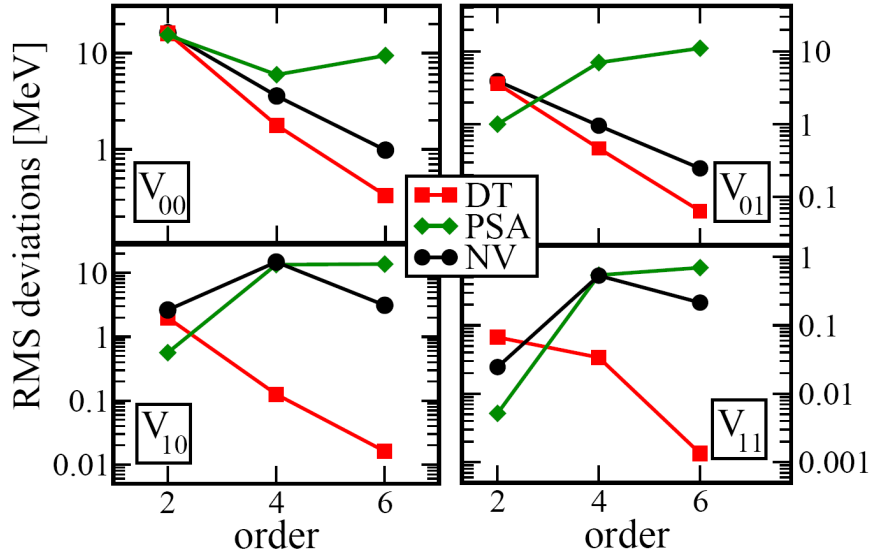
The success and convergence of the DME expansions relies on the fact that the finite-range nuclear effective interactions (G-matrix, Gogny, M3Y,...) are very short-range as compared to the spatial variations of nuclear densities. The quasi-local (gradient) expansion in nuclei works!

B.G. Carlsson & J.D. Phys. Rev. Lett. 105, 122501 (2010)

DME for the Gogny direct energy



DME for the Gogny exchange energy



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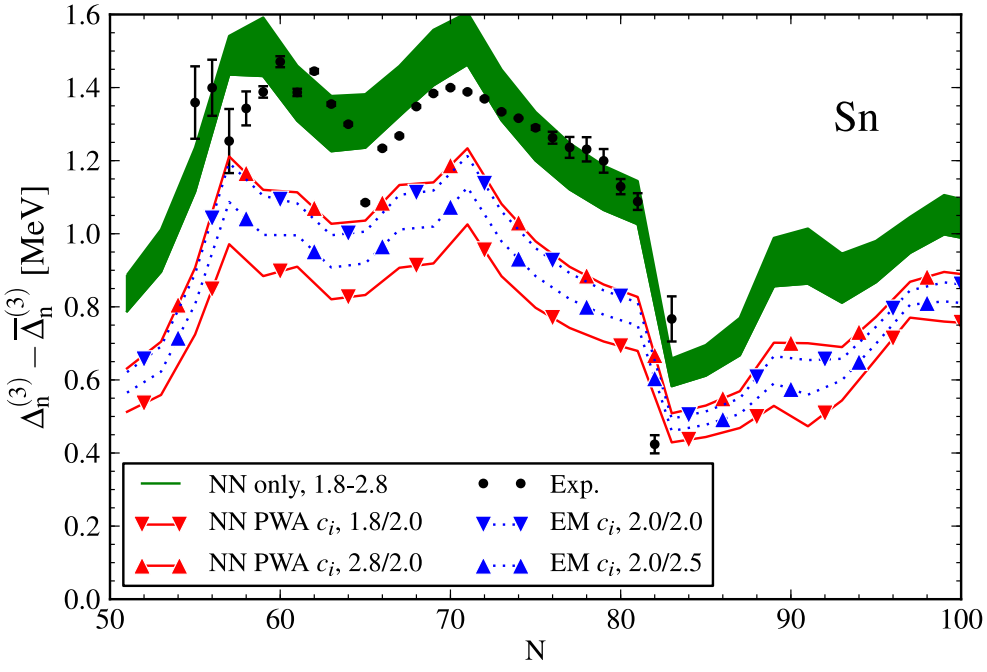
“Chiral three-nucleon forces and pairing in nuclei”

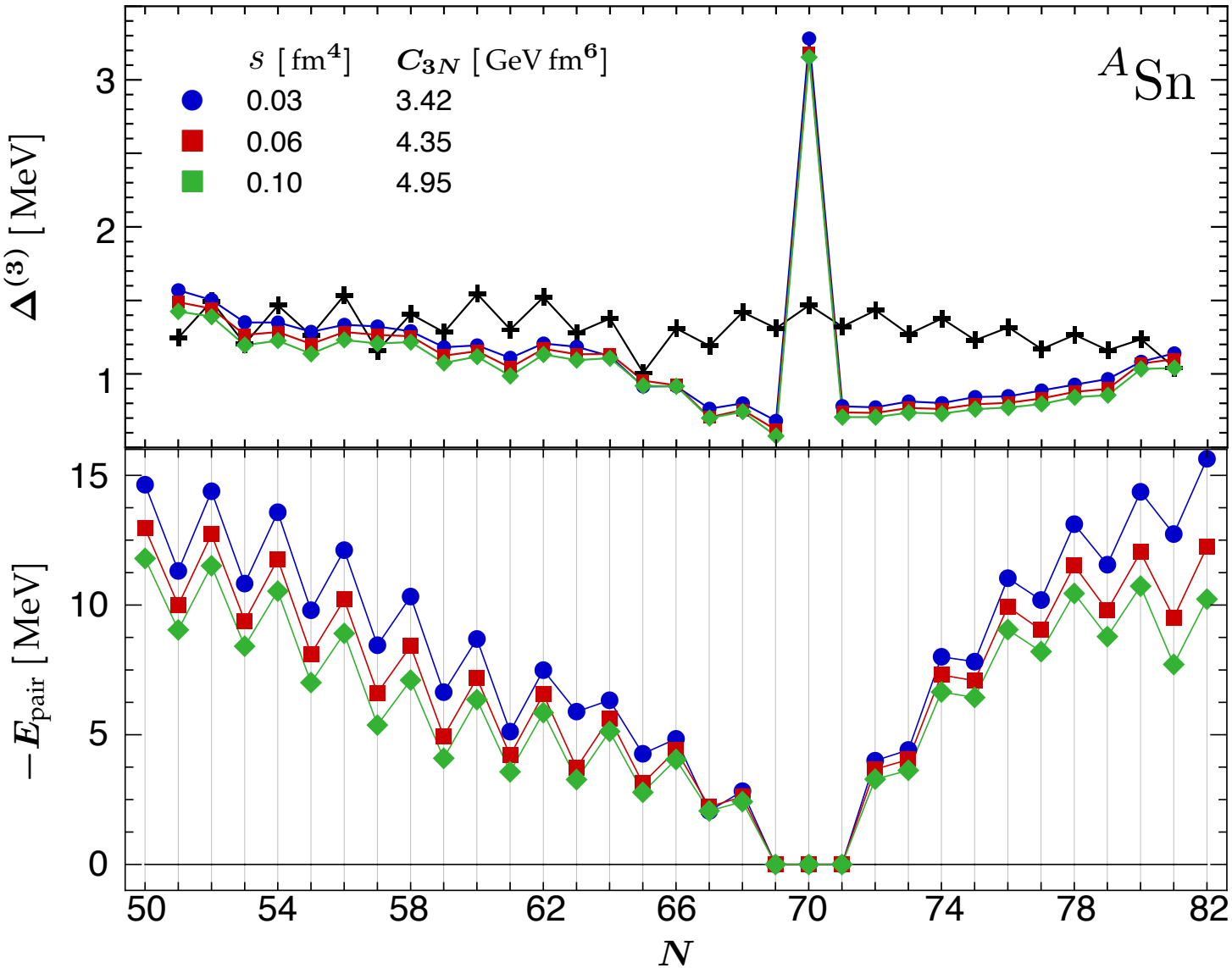
T. Lesinski, K. Hebeler, T. Duguet, A. Schwenk, arXiv:1104.2955

- Uncertainties: 100–200 keV for NN; 100–250 keV for 3N
- short-range higher-order NN and 3N; long-range 3N c_i’s
- 3N needed for quantitative pairing gaps
- 1st-order low-momentum leaves 30% for higher orders



- Next: normal self-energy and higher-order contributions to pairing kernel consistently based on low-momentum NN+3N
- Apply non-empirical pairing EDF to deformed nuclei

Hartree-Fock-Bogoliubov: V_{SRG}+DDI



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Ab-initio inputs fur nuclear functionals

- Typically assume form of functional and fit parameters
- Observables: cannot do better than experiment
- ✔ Theoretical intermediates

- Use Kohn-Sham DFT (formulated for a trapped nucleus) mapped on CCSD
- Adequate for a doubly-magic nucleus
- Start from a g.s. CCSD calculation (^{48}Ca, $V_{\mathrm{low}\ k}$ $\Lambda = 1.9$)
- Construct a functional $\mathcal{E}$ expanded quadratically around CC g.s. density

Summary and outlook

- Progress in many-body techniques and understanding of the nuclear $\hat{H}$ allows to add meaninful input to nuclear functionals
- Kohn-Sham DFT useful in establishing theory vs. theory comparison
- Issues may arise (V-representability, numerics) but technique is promising
- Work with intrinsic densities
- Perform further CC calculations with various external potentials to probe spatial response of KS fields to density variations
- Can also assume analytic functional form and fit parameters at level of potential instead of data
- Self-consistency check: should agree with CC g.s. energy

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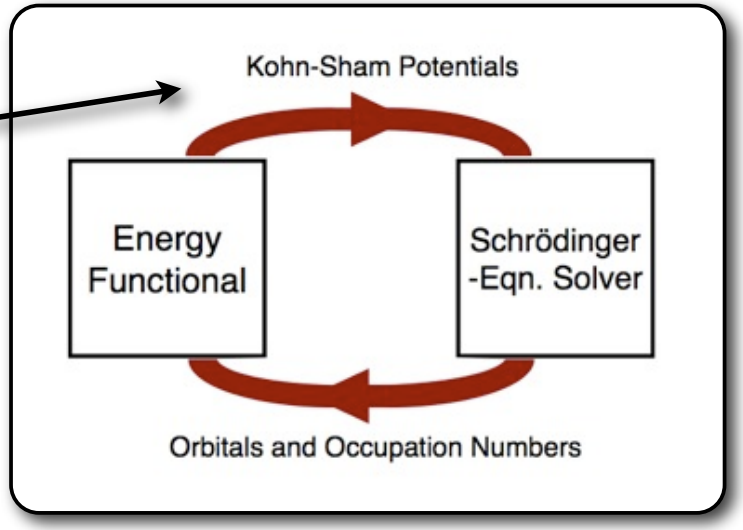
The Optimized Effective Potential

- The OEP is just the KS auxiliary potential. It is called OEP when the functional depends only implicitly on the density and explicitly on the KS orbitals.

So we can't just do this: $$v_{KS}(\mathbf{r}) = \frac{\delta E_{int}[\rho]}{\delta \rho(\mathbf{r})}$$

Instead we have to solve an integral equation to find the potential, but other than that the KS loop remains unchanged.

➡ We need an OEP solver

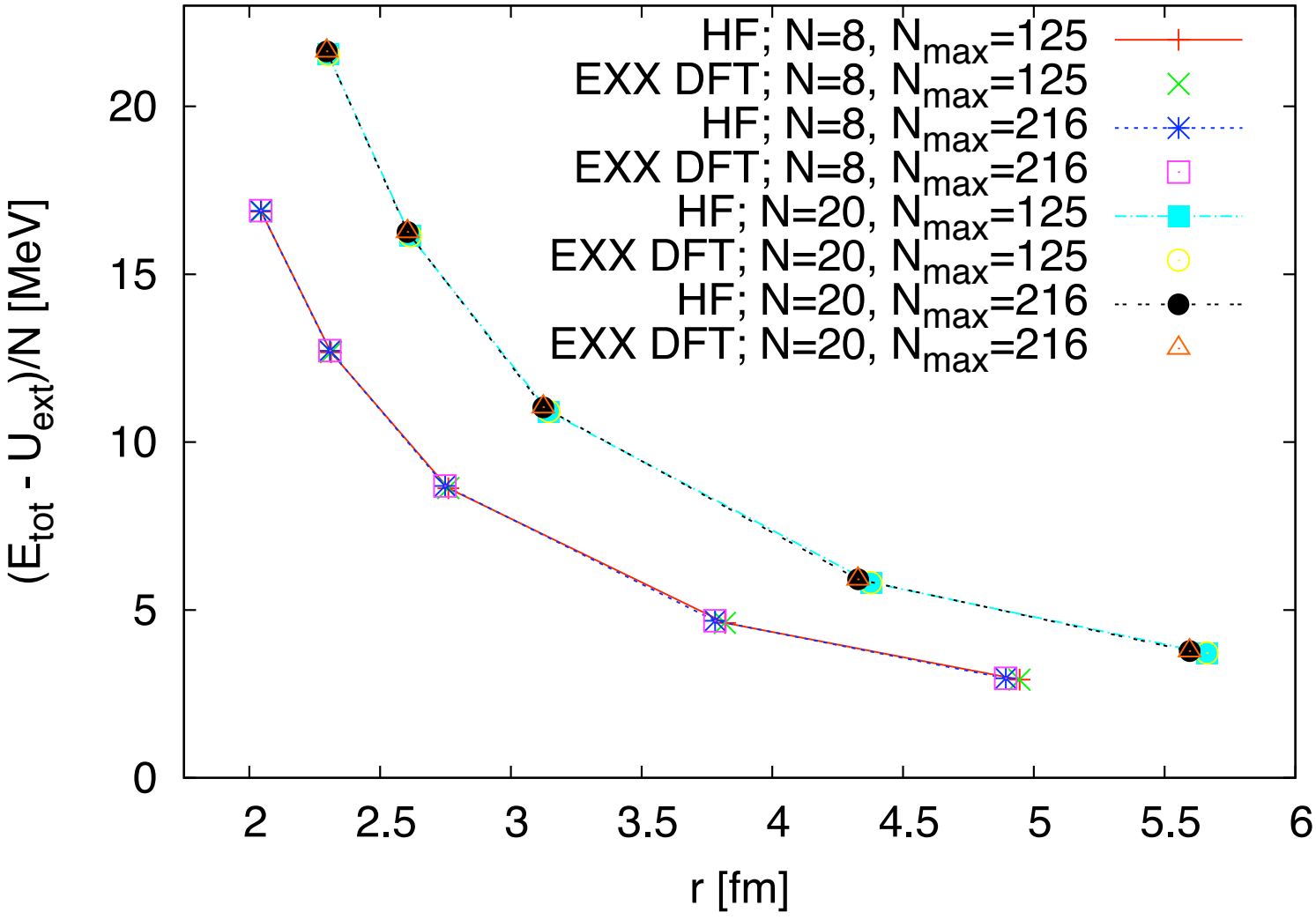


Results

- Neutron drops with the Minnesota interaction
- Various basis sizes and trap frequencies
- Full 3D problem! (no symmetry assumed)
- Exact-exchange (EXX) functional vs. Hartree-Fock
- Solved OEP Eqn. exactly with KP algorithm
- J. E. Drut and L. Platter, [arXiv:1104.4357].
  Under (positive) review in Phys. Rev. C.

Results: Neutron drops

- Internal energy vs. radius J. E. Drut and L. Platter, [arXiv:1104.4357].



Superfluid OEP

$$\sum_k \Psi_k^\dagger(\mathbf{x}) P_\sigma \Phi_k(\mathbf{x}) + \text{c.c.} = 0$$

$$\sum_k \Psi_k^\dagger(\mathbf{x}) P_\Delta \Phi_k(\mathbf{x}) + \text{c.c.} = 0$$

$\Phi_k(\mathbf{x})$ Kohn-Sham orbitals

$\Psi_k^\dagger(\mathbf{x})$ Orbital shifts

We just need to define some projectors:

$$P_\sigma = \begin{pmatrix} \mathbb{1}_\sigma & 0 \\ 0 & -\mathbb{1}_\sigma \end{pmatrix} \qquad P_\Delta = \begin{pmatrix} 0 & i\sigma_2 \\ -i\sigma_2 & 0 \end{pmatrix}$$

$$\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbb{1}_\uparrow = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \mathbb{1}_\downarrow = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Can we apply the KP algorithm here?

Done / To-do update

- Implemented full **OEP** solution in 1D (Kümmel-Perdew algorithm) ✔
  - Allows for orbital-dependent functionals
  - Solves formal and practical problems of GGAs
  - Allows for exact exchange, RPA, Pairing, etc...
- Tested 1D proof-of-concept against Hartree-Fock ✔
- Derived Superfluid OEP equations (first time) ✔
- Tested EXX-DFT versus HF for 3D neutron drops with Minnesota interaction. (first time a spin-dependent potential is OEP'd!)
  J. E. Drut and L. Platter, [arXiv:1104.4357]. ✔
- Improved Superfluid-OEP formalism ✔
- Coded Superfluid OEP ✔
  (all parts in place, KP algorithm seems to fail in this case)

What's next?

- We have performed test calculations for the OEP with 3-body forces at the EXX level. The corresponding formalism is easy to derive. It remains to write this up and post it.
- We need to extend this to higher-body forces. The formalism is easy at the EXX level.
- We need a Superfluid OEP solver.
- Proceed towards using low-momentum potentials.
- Continue to pursue higher-order functionals (with 2-body forces for now)
- Is there a useful KLI approximation in the superfluid case?
- RPA? QRPA?

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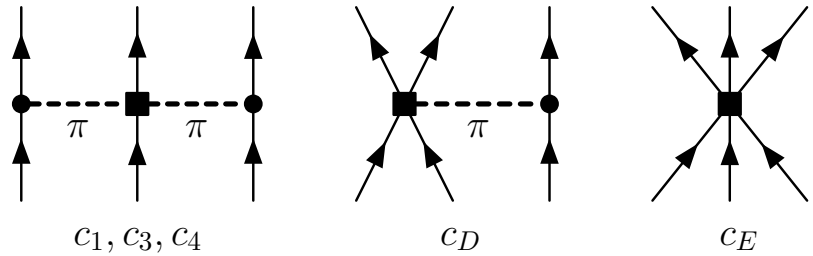
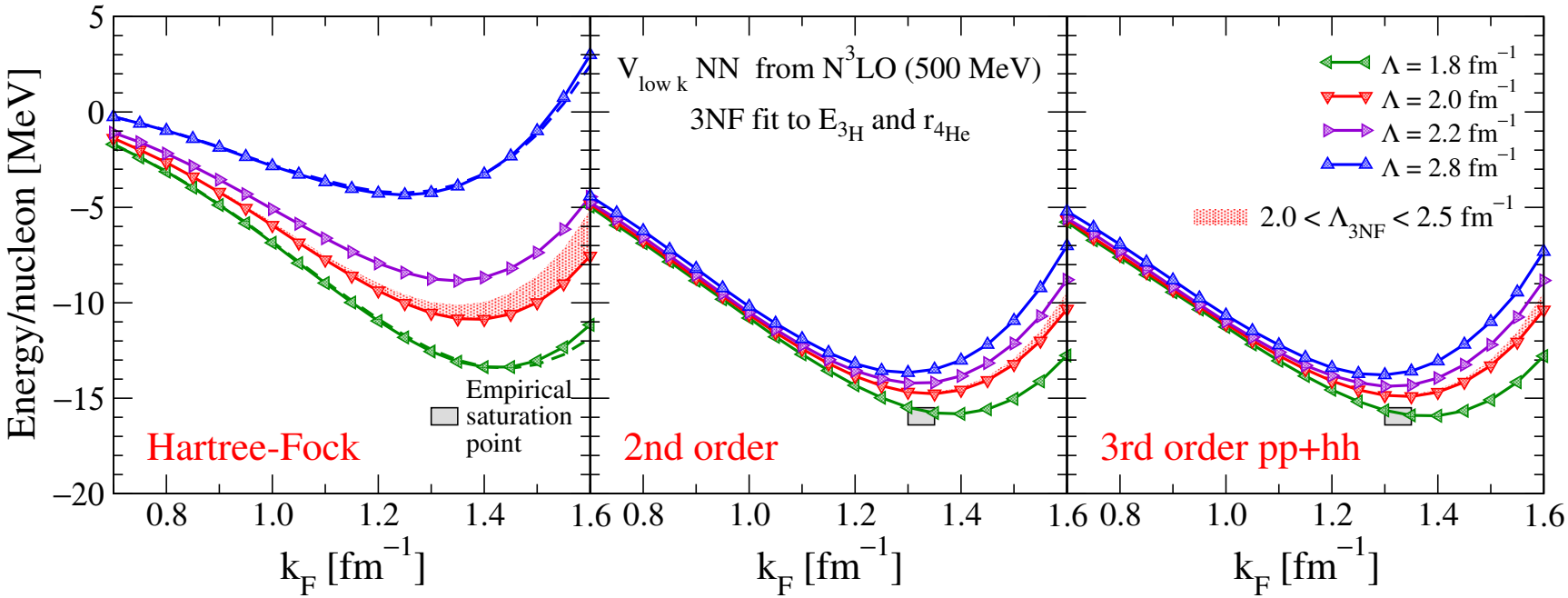
"Improved nuclear matter calculations from chiral low-momentum interactions"

K. Hebeler, S.K. Bogner, R.J. Furnstahl, A. Nogga, and A. Schwenk, Phys. Rev. C 83, 031301 (2011)

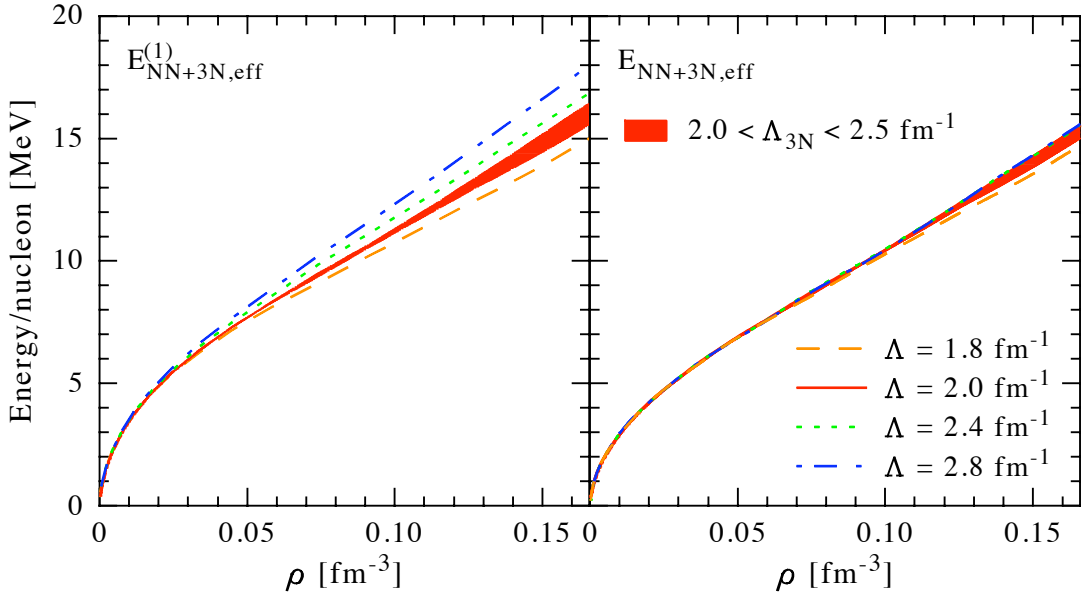
- Evolve Λ down with RG (to $\Lambda \approx 2\,\mathrm{fm}^{-1}$ for ordinary nuclei)
  - NN interactions fully, NNN interactions approximately
- Fit two 3NF constants to triton binding and ^{4}He radius
  $\Longrightarrow$ predict nuclear matter

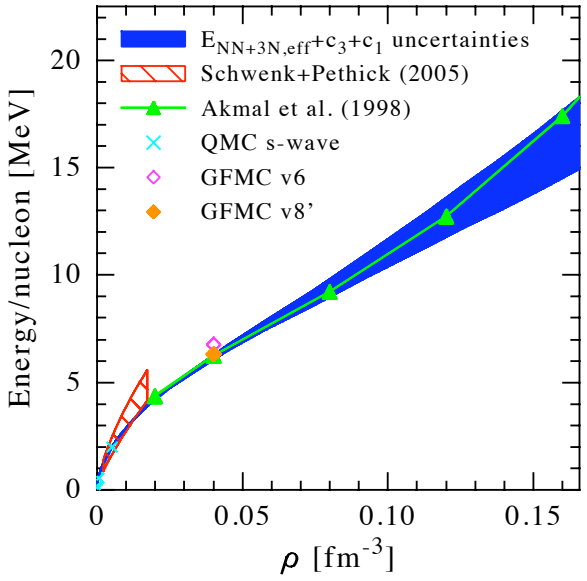


Use effective $\overline{V}_{3N}$ in MBPT



Application to neutron matter and neutron stars





KH and A. Schwenk PRC 82, 014314 (2010)

- Significantly reduced cutoff dependence at 2nd order
- Energy sensitive to long-range 3NF c_3 variations
- Good agreement with other approaches (different NN)

Ab Initio Nuclear DFT Deliverables

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- SRG: develop few-body operators, test factorization, explore alternative generators to control many-body operators

Personnel

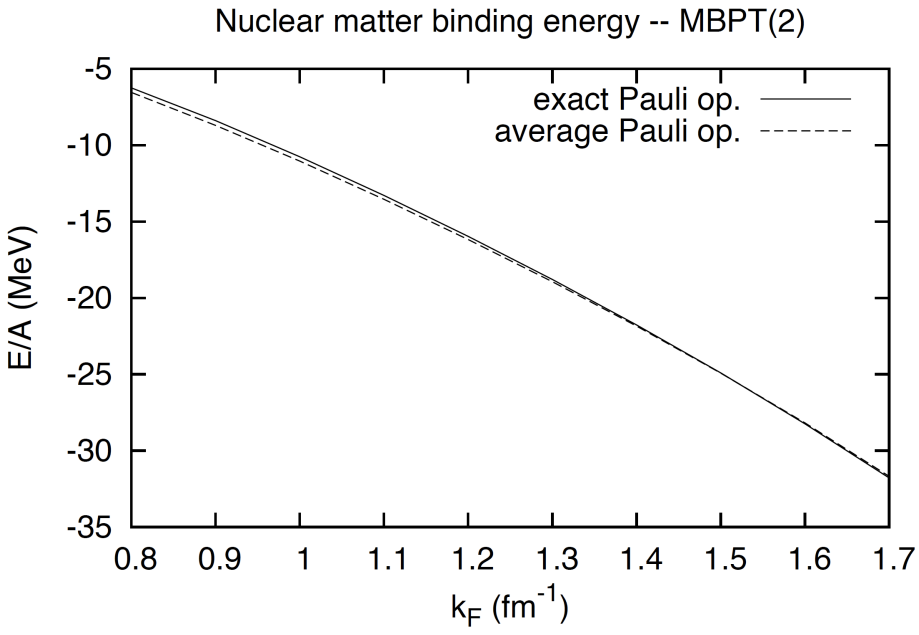
UNEDF collaborators: G. Hagen, J. Holt, T. Papenbrock, T. Lesinski (UW)

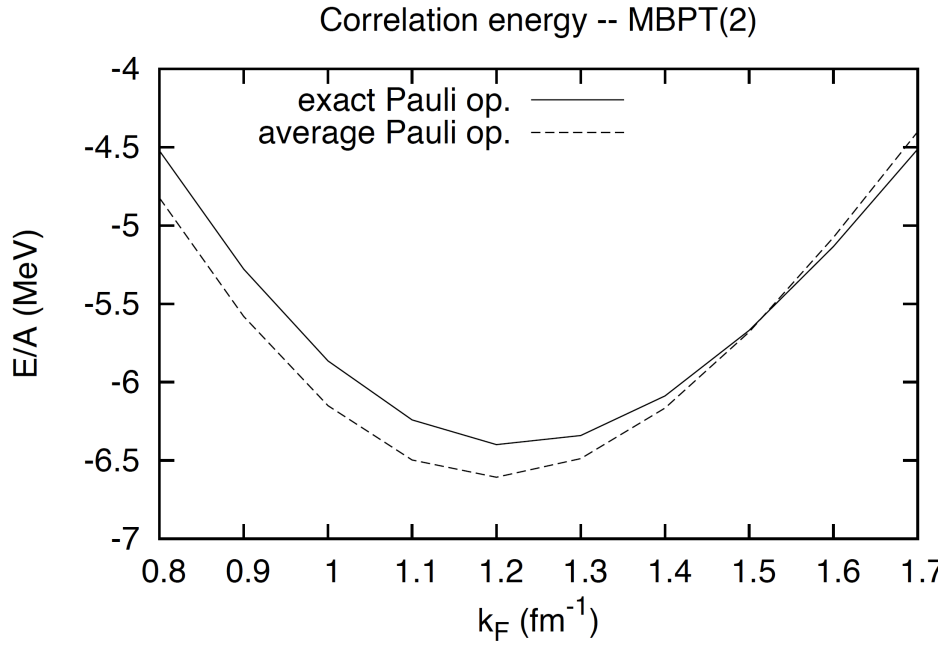
CS support: Hai Ah Nam (ORNL)

Development of coupled-cluster method with relevance for UNEDF (by students supervised by M. Hjorth-Jensen and G. Hagen)

- Øyvind Jensen (student at University of Bergen – Graduated July 2011; one-nucleon overlap functions and spectroscopic factors in J-coupled scheme)
- Gustav Jansen (student at University of Oslo; closed shell ±2 nucleons)
- Gustav Baardsen (student at University of Oslo; coupled-cluster theory for infinite nuclear matter)

Coupled-cluster theory for nuclear matter (Preliminary)





Implemented exact Pauli operator in relative-center of mass coordinates
Implemented Hartree-Fock and MBPT(2) for nuclear matter in relative and Center-of-mass coordinates. Code has been validated and verified using Argonne-V18 and vlow-k.

Particle-particle and hole-hole ladders are in progress.
Particle-hole channels will be implemented using exact and angle average Pauli operator

Things in progress

- SRG connections between chiral and pionless EFT.
- Hyper-radial momentum space evolutions for A>3.
  - Test of low momentum universality in 3D for A-body forces.
  - Visualization of SRG evolution beyond A>3.
- Extend local projection analysis to A>2.
  - Find and use other local “projections”.
- Continue work on controlling induced 4-body forces (from initial 3-body)
- QMC methods for chiral/srg interactions
  - Ψ is simple after SRG (correlations suppressed)
  - Non-local makes other things harder (lots of spectator and conservation delta functions to handle, etc)
  - VMC Soon, LR-DMC later.

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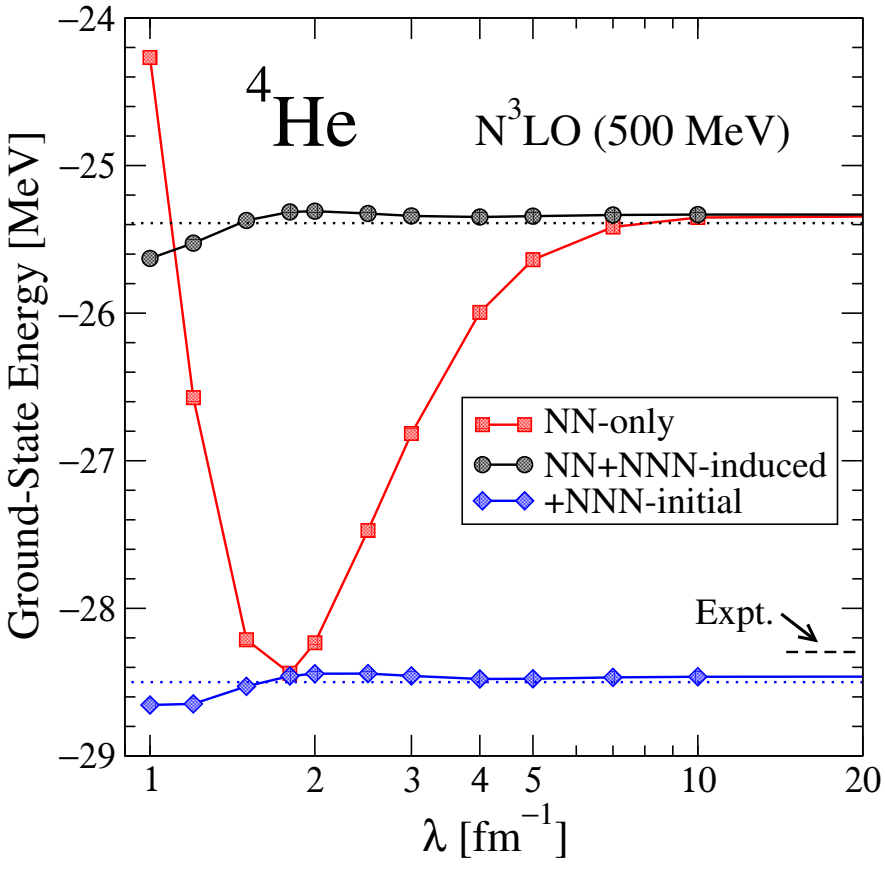
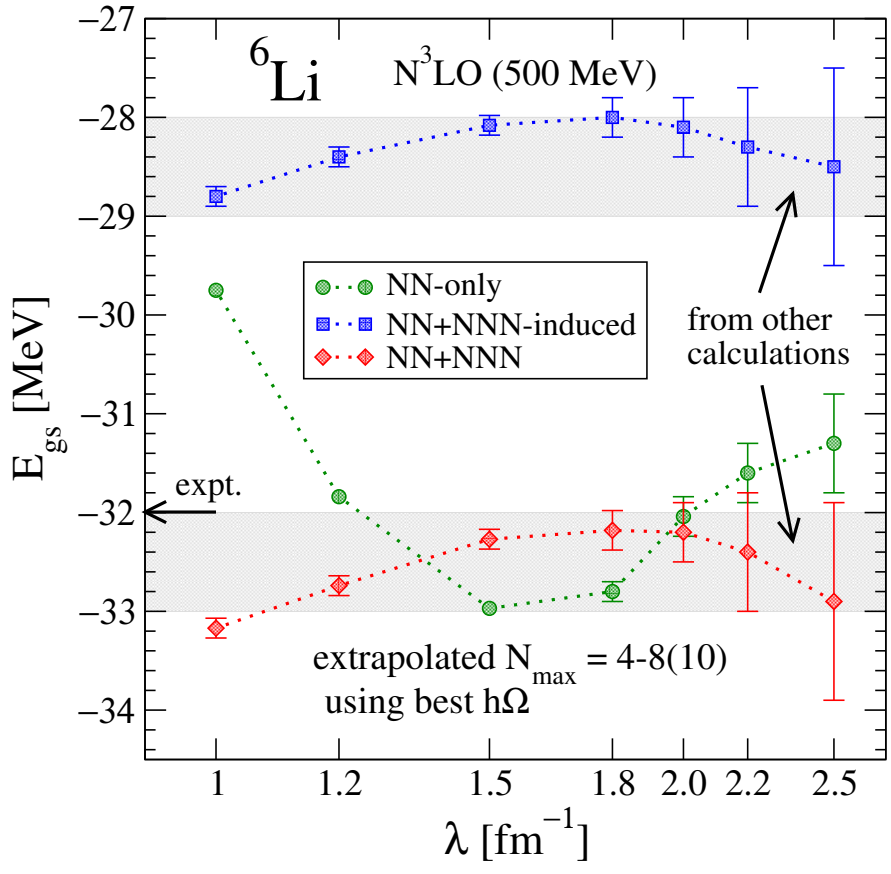
"Evolving nuclear many-body forces with the SRG"

E.D. Jurgenson, P. Návratil, R.J. Furnstahl, Phys. Rev. C 83, 034301 (2011)

- Look at running of ^{4}He and ^{6}Li energy with λ



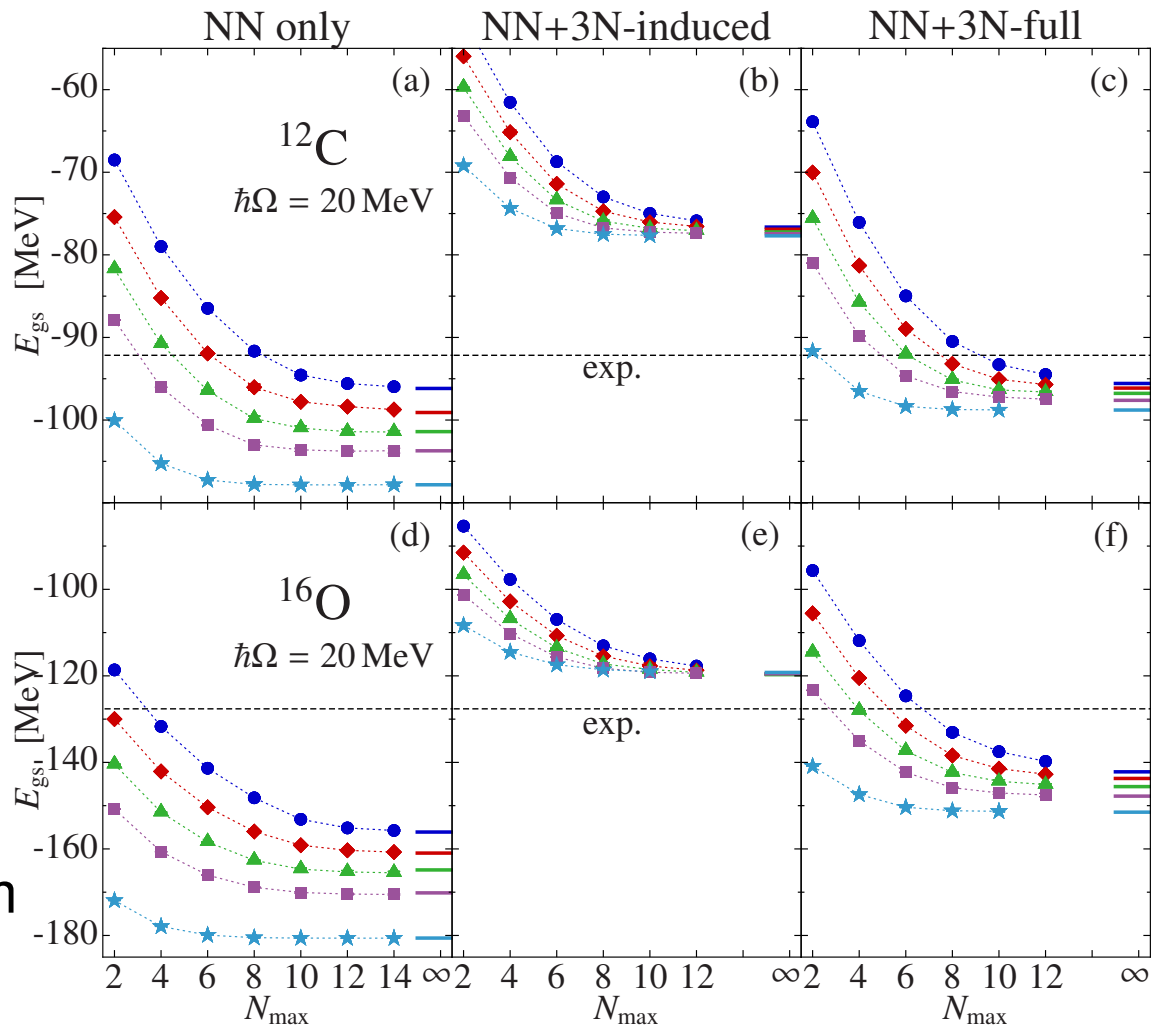


- Manifest induced 4NF but same whether initial 3NF or not
- What about the *A* dependence? No problem up to ^{6}Li

"Similarity-transformed chiral NN+3N interactions for the ab initio description of 12-C and 16-O"

R. Roth, J. Langhammer, A. Calci, S. Binder, P. Navrátil, arXiv:1105.3173v1

- SRG evolved in HO basis
- Importance-truncated NCSM $\Longrightarrow$ larger $N_{\max}$
- Here: $E_{\rm gs}$ vs. $N_{\max}$
- NN-only is not unitary
- NN+3N-induced is still unitary
- NN+3N-full spreads $\Longrightarrow$ significant 4NF (confirmed by Jurgenson)
- Small spread for spectrum



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3NF Evolution Progress and Plan [K. Hebeler]

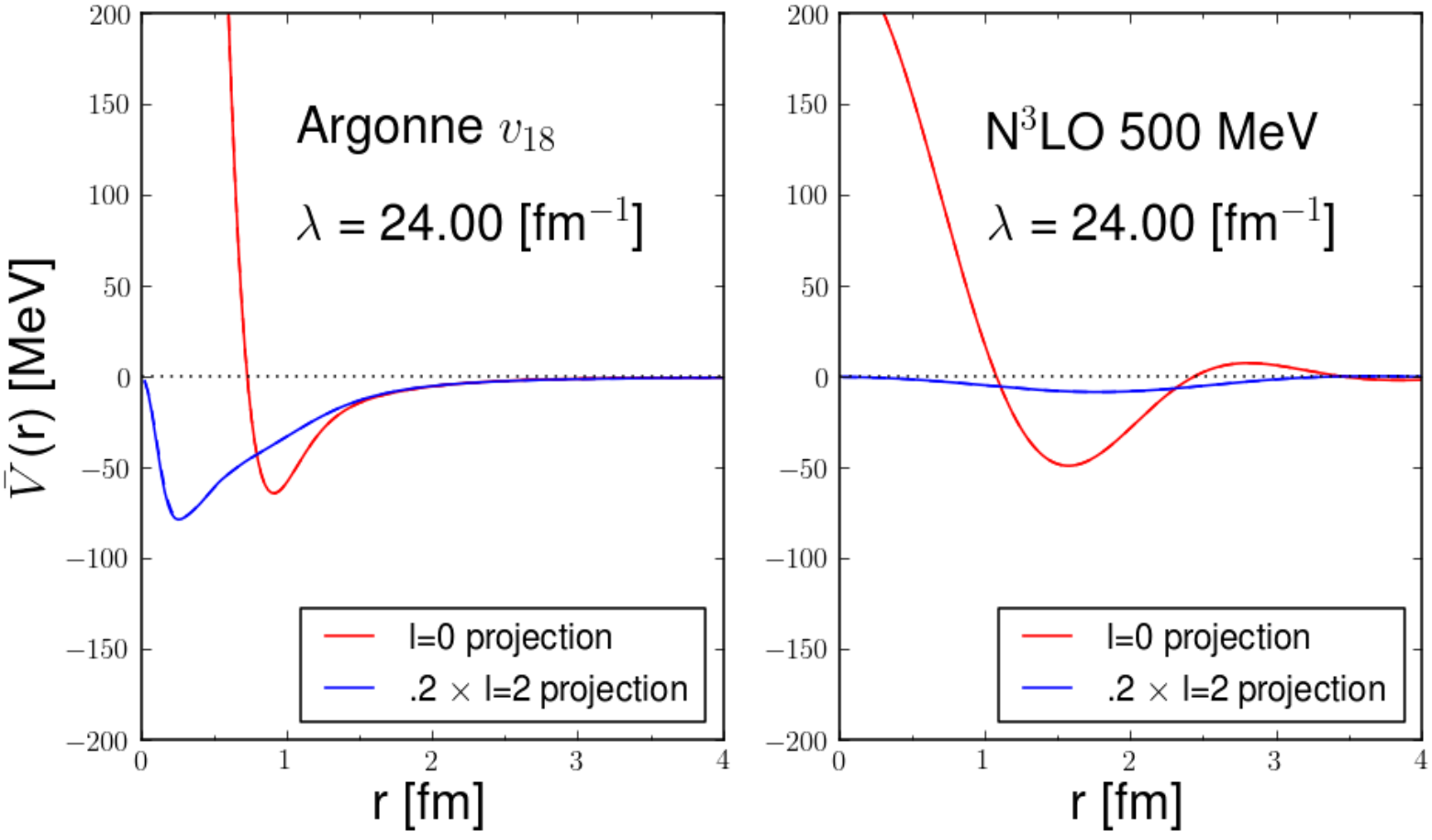
- $A = 3$ Faddeev code written from scratch (NN-only so far)
  - Extend to include 3NF
- Right side of SRG differential equations for V_{123} evolution
  - Expressions recently derived
  - Coded but not fully tested (uses OpenMP $\Longrightarrow$ add MPI)
  - Improve efficiency (suggestions?)
- Computational issues
  - Many coupled first-order differential equations:

$$|p\,q\,\alpha\rangle \quad \Longrightarrow \quad (\#\,p \text{ points}) \times (\#\,q \text{ points}) \times (\alpha \text{ partial wave sum})$$

    with $15 \le p \le 40$, $10 \le q \le 25$, $5 \le \alpha \le 34$
  - At each step in s, right side matrix elements each have up to 4 internal loops besides 6 external loops over $p, p', q, q', \alpha, \alpha'$
- Test using Faddeev code and against 3NF HO evolution
- Apply to HF (and beyond) for infinite matter

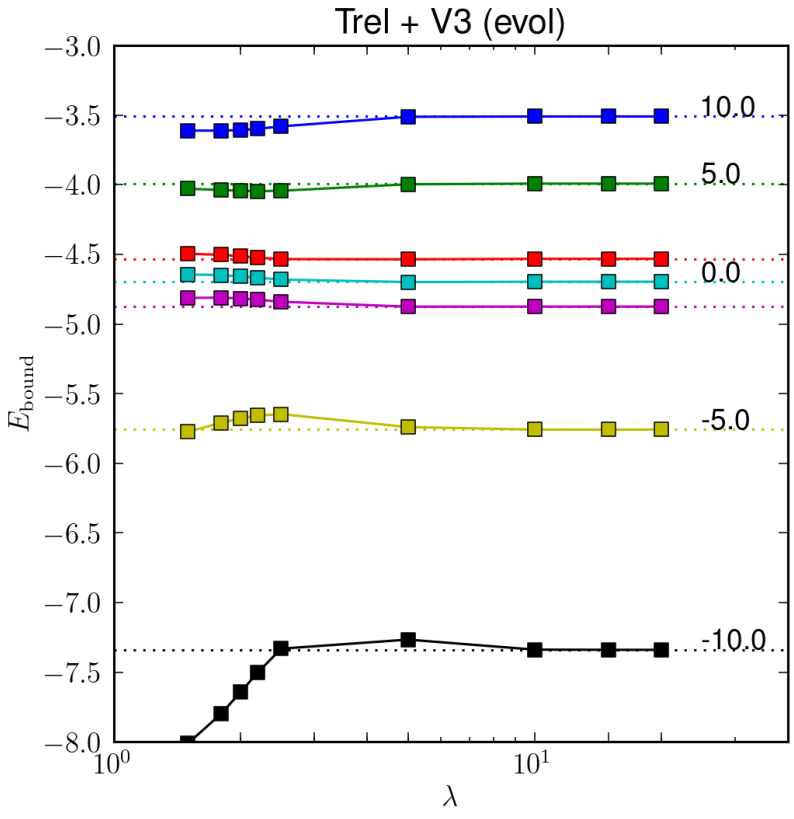
SRG Effects at Long Range: Local Projections

[from Kyle Wendt's talk]

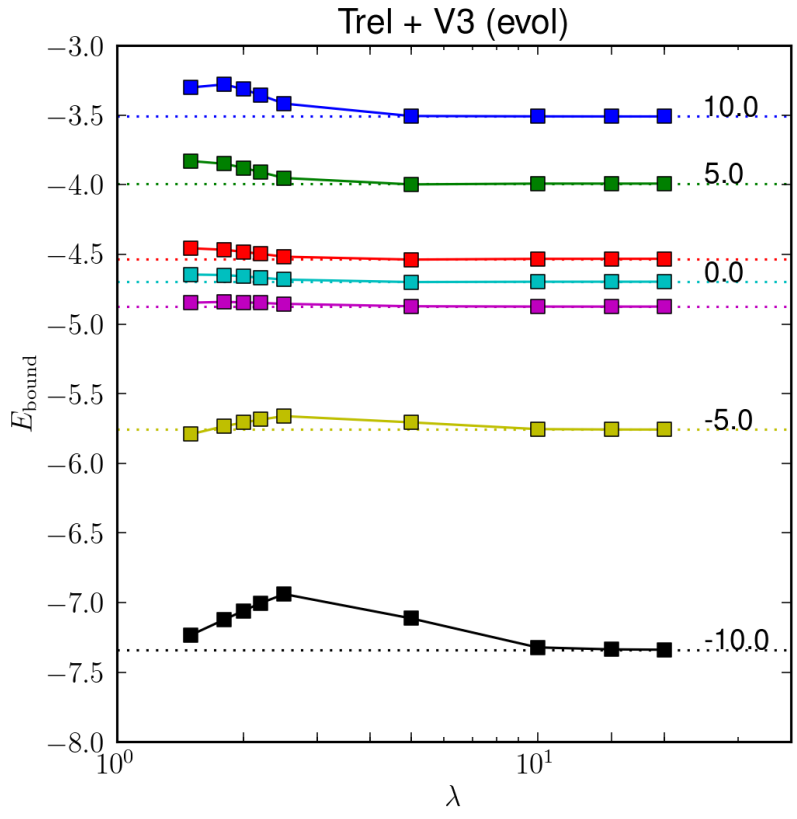


Manipulation of the Evolution of the Three Body Force

$$\frac{d}{ds}H = [[T_{rel} + V_s^{(3)}, H], H]$$



$$\frac{d}{ds}H = [[T_{rel} - V_s^{(3)}, H], H]$$



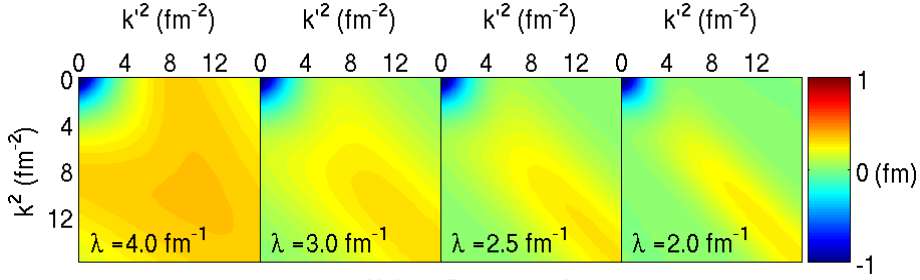
The Similarity Renormalization Group with Novel Generators

W. Li, era, and R.J. Furnstahl, arXiv:1106.2835v1 [nucl-th].

- **The Similarity Renormalization Group (SRG)**

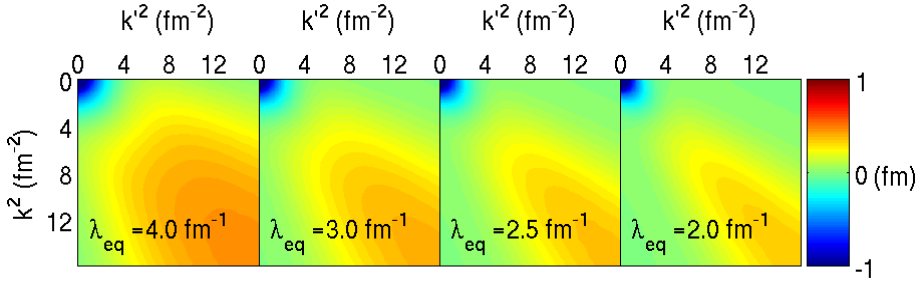
$$\frac{dH_s}{ds} = [\eta_s, H_s] = [[G_s, H_s], H_s]$$

Typically, $G_s = T_{\rm rel}$ with $\lambda = \frac{1}{s^{1/4}}$ fm^{-1}

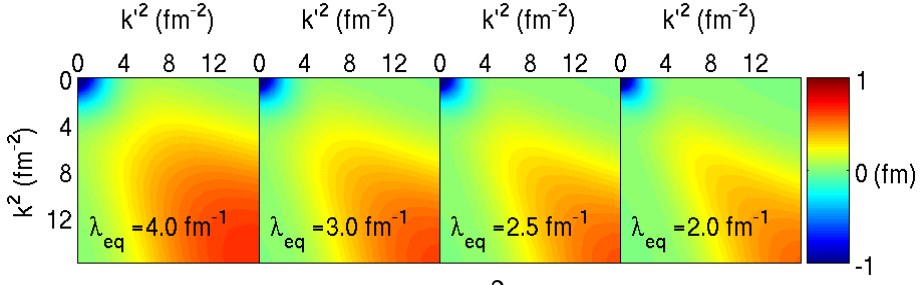


AV18 Potential

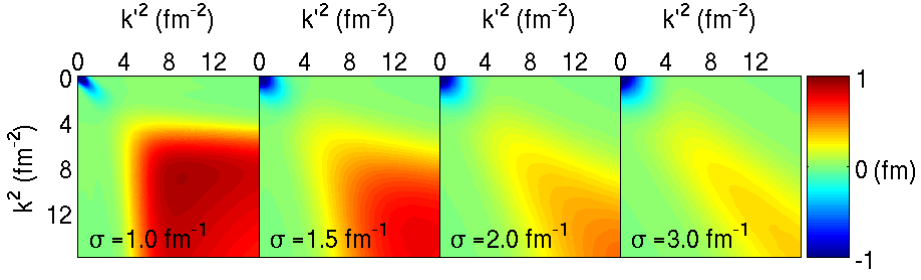
- **SRG flow can be tailored with alternative choices of G_s**
  - λ_{eq} redefined to match decoupling
- Using $G_s^{\rm exp}$ and $G_s^{\rm inv}$ with $\sigma = 2\,{\rm fm}^{-1}$, low E part of V still decoupled
- Much less evolution at high E
  $\Rightarrow$ much faster!



$$G_s^{\rm inv} = -\sigma^2/(1 + T/\sigma^2) \approx c + T + \cdots$$

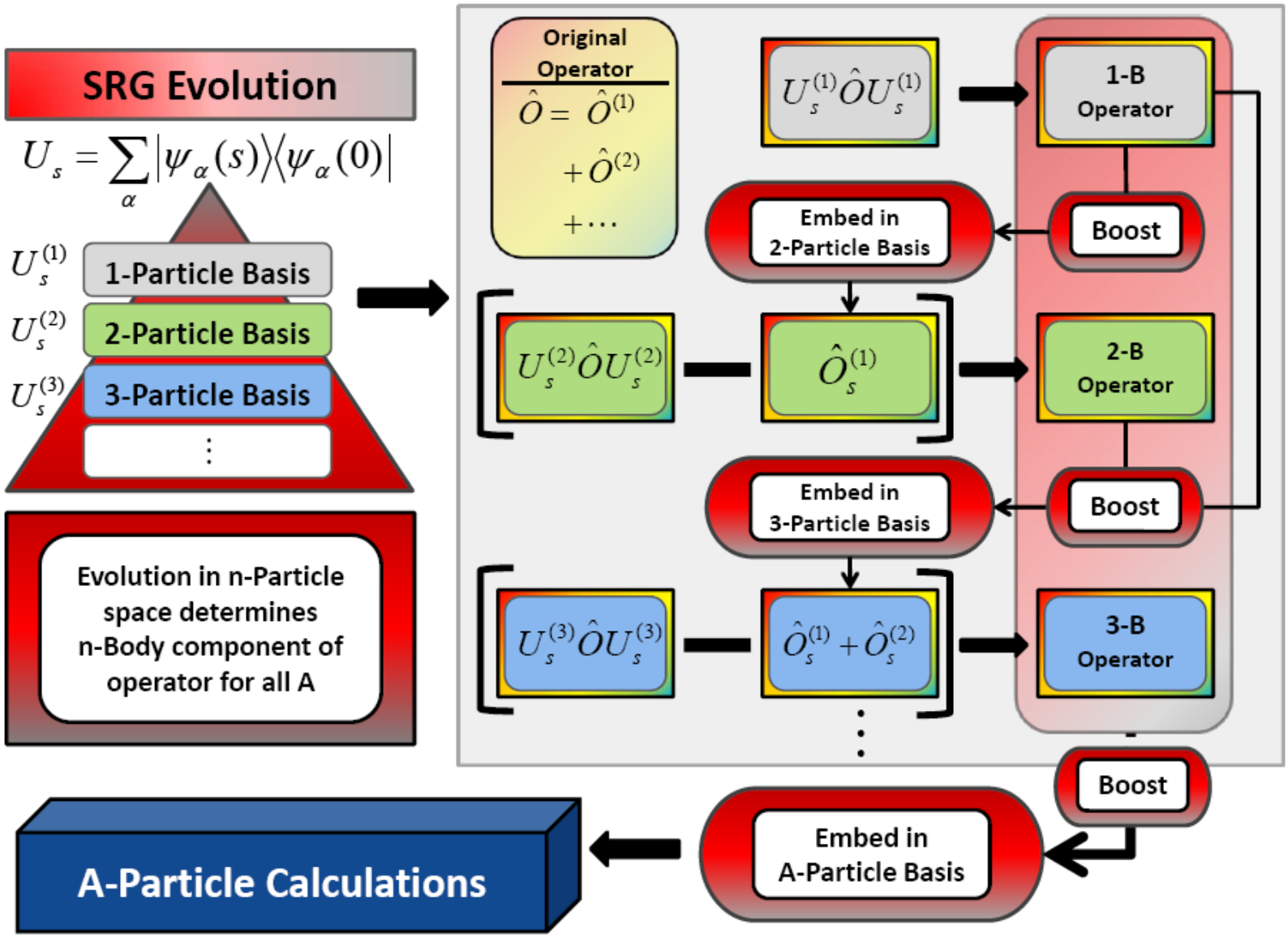


$$G_s^{\rm exp} = -\sigma^2 e^{-T/\sigma^2} \approx c + T + \cdots$$

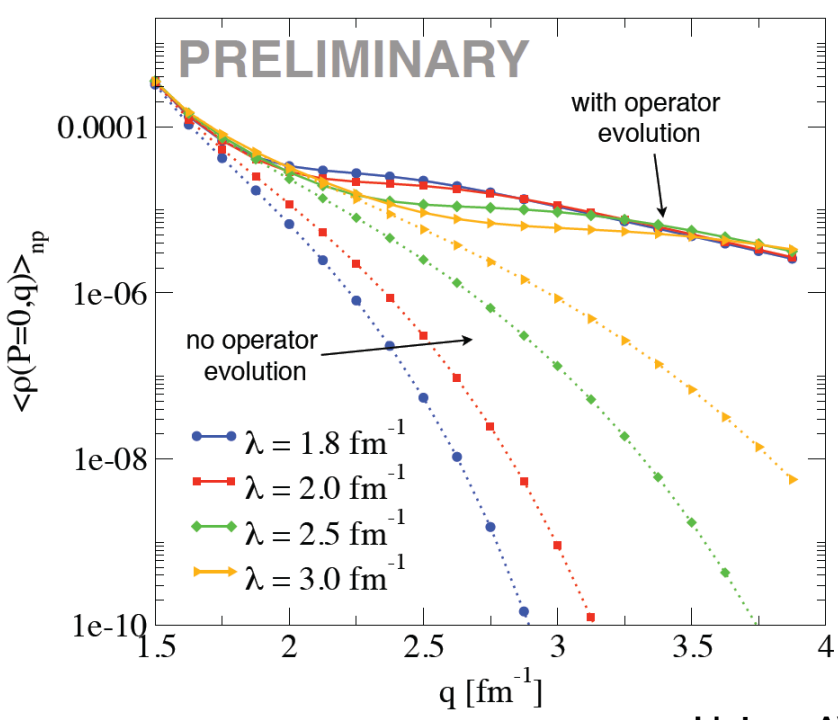


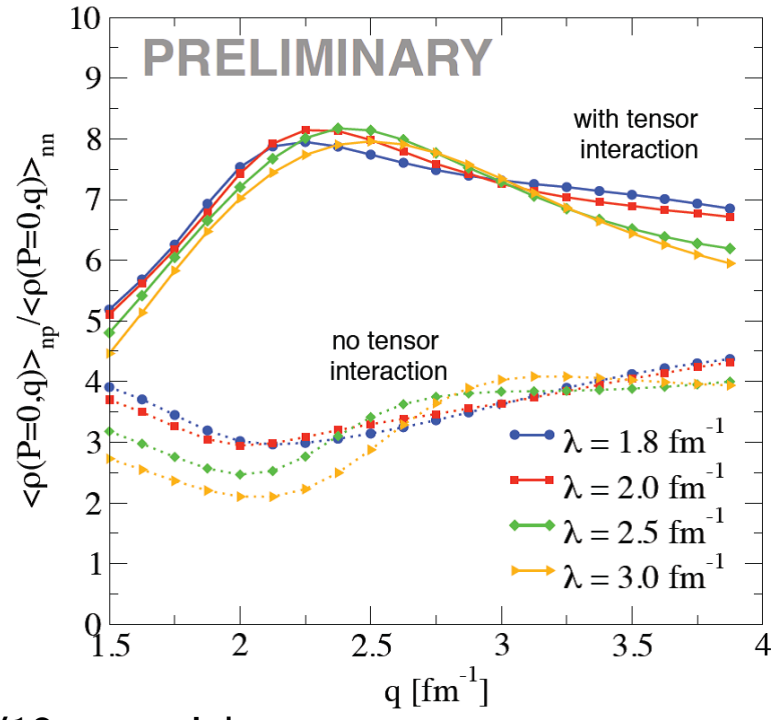
Same $\lambda_{\rm eq} = 2\,{\rm fm}^{-1}$: σ controls pattern.

Operator Evolution & Extraction Process



SRG Evolution of Operators in Nuclear Matter





Using AV18 potential

- Pair-densities are approximately resolution independent
- Enhancement of *np* over *nn* pairs due to tensor force
- To do: Compare to finite nuclei results with LDA

Work done with K. Hebeler

Factorization: Evidence & Use

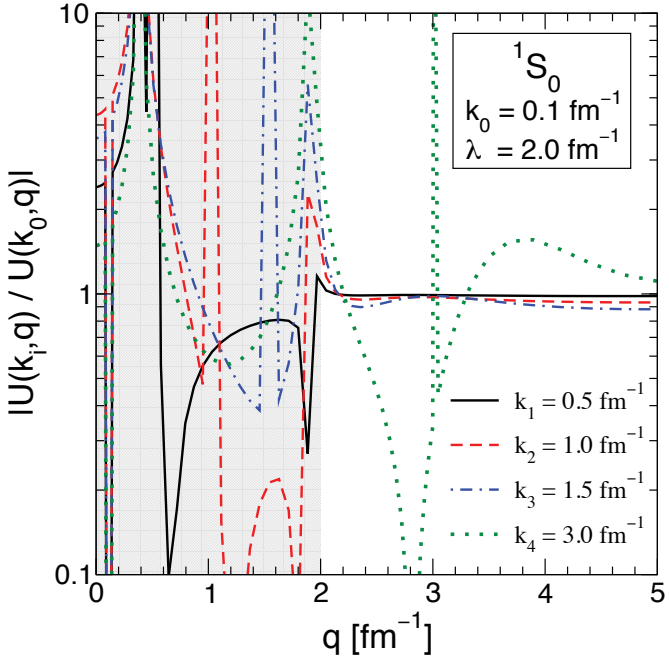
Idea: If $k < \lambda$ and $q \gg \lambda \Longrightarrow$ **factorization**: $U_\lambda(k,q) \to K_\lambda(k) Q_\lambda(q)$

- A **test of factorization** in U can be made by assuming

$$\frac{U_\lambda(k_i,q)}{U_\lambda(k_0,q)} \to \frac{K_\lambda(k_i) Q_\lambda(q)}{K_\lambda(k_0) Q_\lambda(q)},$$

  so for $q \gg \lambda \Rightarrow \frac{K_\lambda(k_i)}{K_\lambda(k_0)}$, if $k < \lambda$.

- As shown below, one can infer this behavior from the plateaus for $q \gtrsim 2\text{fm}^{-1}$ when $k_i < \lambda$



- Motivated by Operator Product Expansion
  - leading OPE predicts $K(k) \sim const$ for s-waves $\Rightarrow$ plateaus at 1
- Using **Factorization**, one finds:

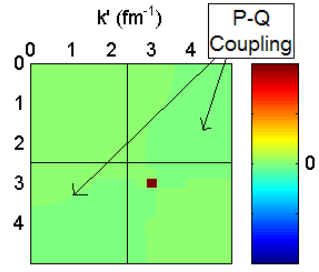
$$\langle \psi_\lambda |\, U_\lambda O\, U_\lambda^\dagger \,| \psi_\lambda \rangle \cong {}^{\lambda}_{0}\langle \psi_\lambda^\dagger(k') |\, {}^{\lambda}_{0}U_\lambda(k',q')\, {}^{\lambda}_{0}O(q',q)\, {}^{\lambda}_{0}U_\lambda(q,k) \,| \psi_\lambda(k) \rangle + {}^{\lambda}_{0}\langle \psi_\lambda^\dagger(k') |\, I_{QOQ}\, K_\lambda(k') K_\lambda(k) \,| \psi_\lambda(k) \rangle$$

  where

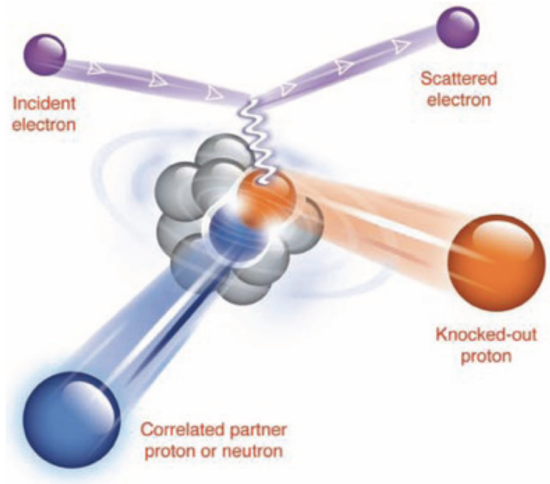
$$I_{QOQ} = \int_\lambda^\infty dq' \int_\lambda^\infty dq \;\; Q_\lambda(q') O(q',q) Q_\lambda(q)$$

  is a *universal* function for all nuclei

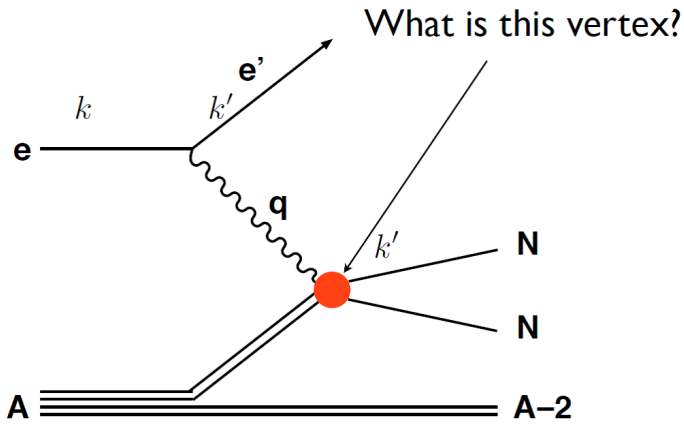
  – *Valid* when initial operators *weakly couple high and low momentum*



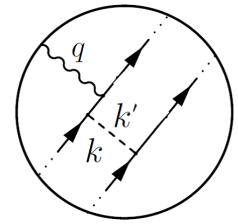
Correlations in Nuclear Systems



Subedi et al., Science 320,1476 (2008)



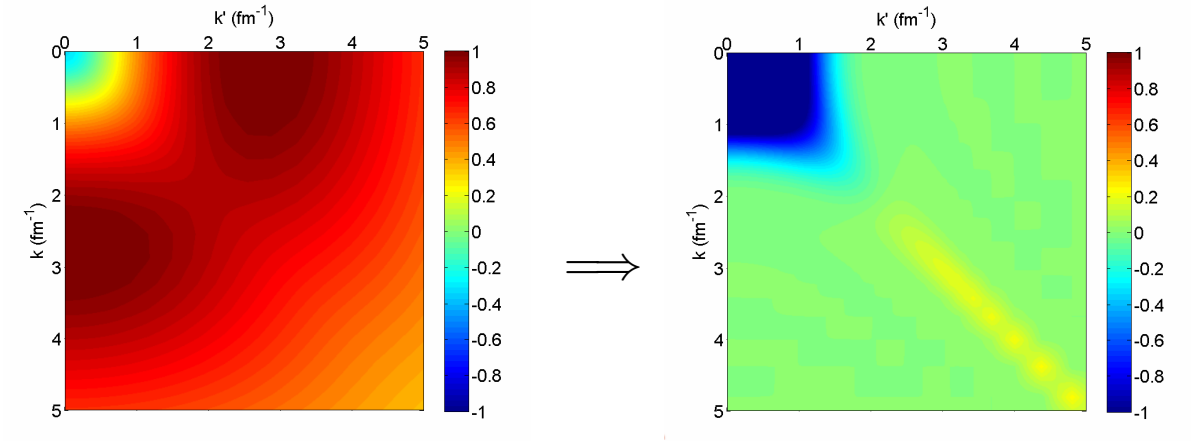
Higinbotham, arXiv:1010.4433



k : low rel. momentum

k' : high rel. momentum

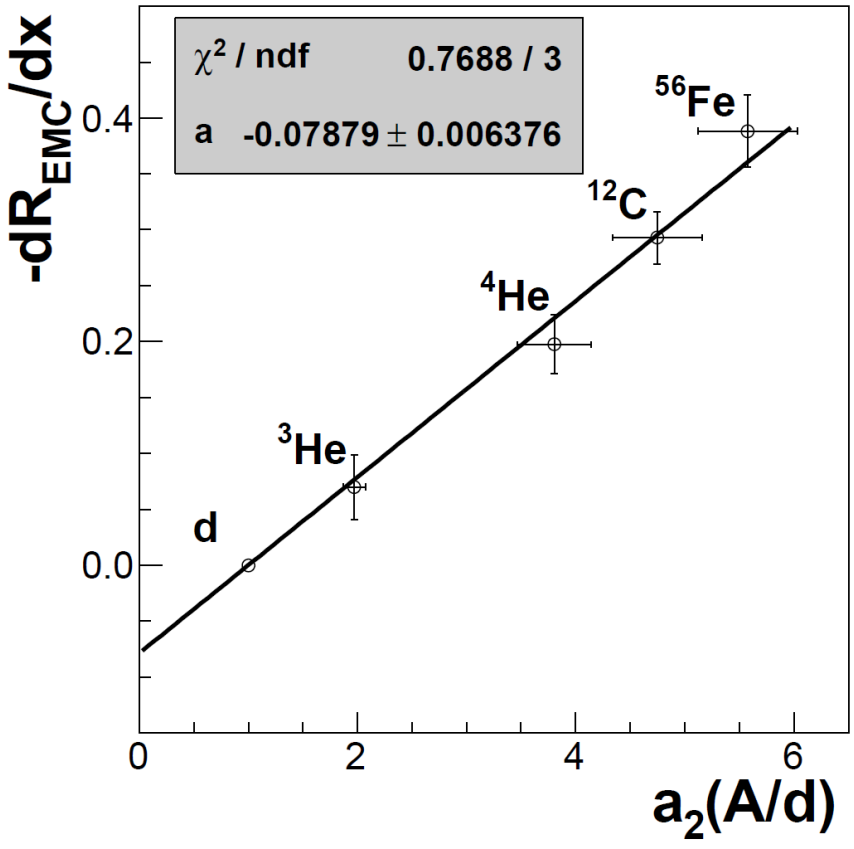
- E.g.: Detection of knocked out pairs with large relative momenta
- How is vertex modified?
- How Understand in Context of SRG and low-momentum interactions?



Short Range Correlations and the EMC effect

- Deep inelastic scattering ratio at $Q^2 \geq 2\,\mathrm{GeV}^2$ and $0.35 \leq x_B \leq 0.7$ and inelastic scattering at $Q^2 \geq 1.4\,\mathrm{GeV}^2$ and $1.5 \leq x_B \leq 2.0$

- Strong linear correlation between slope of ratio of DIS cross sections (nucleus A vs. deuterium) and nuclear scaling ratio



L.B. Weinstein, et al., Phys. Rev. Lett. 106, 052301 (2011)

Can nuclear scaling and EMC effect be explained via factorization of operators and low momentum structure of the nuclei?

- We can calculate a_2 in MBPT
- Same dependence on nuclear structure for high momentum operators
  $\Rightarrow$ EMC effect?

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MSU Year 5 Status Report

I) Density Matrix Expansion/ab-initio EDFs

see M. Kortelainen's talk

Scott Bogner
Juan Burgos (student)

II) In-medium SRG

Scott Bogner
Heiko Hergert
Koshiroh Tsukiyama**
Achim Schwenk**

**External

Year 5 papers with UNEDF support

1. "Testing the density matrix expansion against ab initio calculations of trapped neutron drops"
   S. K. Bogner, R. J. Furnstahl, H. Hergert, M. Kortelainen, P. Maris, M. Stoitsov and J. P. Vary
   arXiv:1106.3557 [nucl-th] SPIRES entry

2. "Improved nuclear matter calculations from chiral low-momentum interactions"
   K. Hebeler, S. K. Bogner, R. J. Furnstahl, A. Nogga and A. Schwenk
   Phys. Rev. C **83**, 031301 (2011) [arXiv:1012.3381 [nucl-th]] SPIRES entry

3. "Microscopically-based energy density functionals for nuclei using the density matrix expansion: Implementation and pre-optimization"
   M. Stoitsov, M. Kortelainen, S. K. Bogner, T. Duguet, R. J. Furnstahl, B. Gebremariam and N. Schunck
   Phys. Rev. C **82**, 054307 (2010) [arXiv:1009.3452 [nucl-th]] SPIRES entry

4. "Operator Evolution via the Similarity Renormalization Group I: The Deuteron"
   E. R. Anderson, S. K. Bogner, R. J. Furnstahl and R. J. Perry
   Phys. Rev. C **82**, 054001 (2010) [arXiv:1008.1569 [nucl-th]] SPIRES entry

5. "In-Medium Similarity Renormalization Group for Nuclei"
   K. Tsukiyama, S. K. Bogner and A. Schwenk
   arXiv:1006.3639 [nucl-th] SPIRES entry (accepted to PRL)

6. "Microscopically-constrained Fock energy density functionals from chiral effective field theory. I. Two-nucleon interactions"
   B. Gebremariam, S. K. Bogner and T. Duguet
   Nucl. Phys. A **851**, 17 (2011) [arXiv:1003.5210 [nucl-th]] SPIRES entry

Normal Ordered Hamiltonians

$$H = \sum t_i a_i^\dagger a_i + \frac{1}{4}\sum V^{(2)}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{36}\sum V^{(3)}_{ijklmn} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l$$

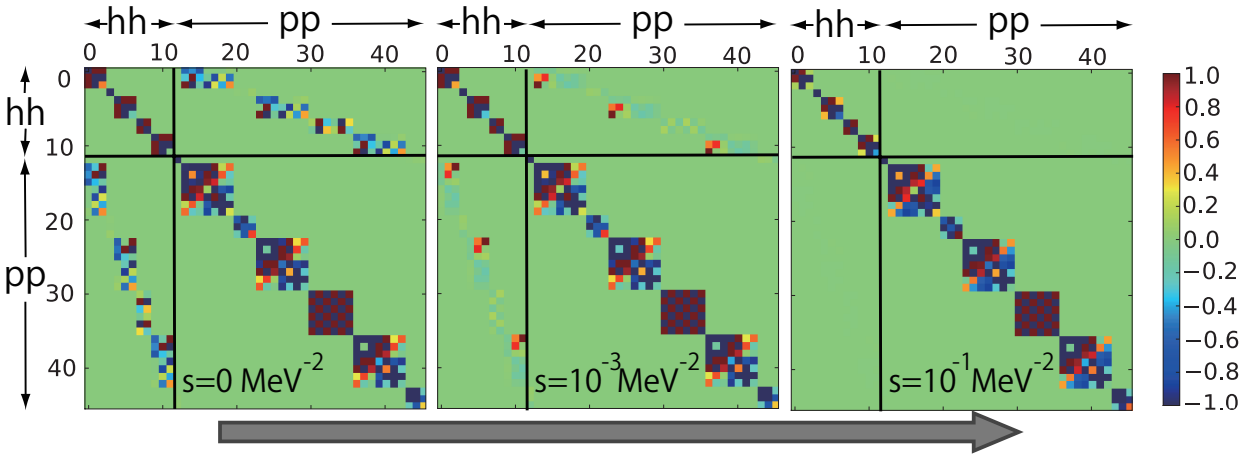
Normal-order w.r.t. some reference state Φ (e.g., HF) :

$$H = E_{vac} + \sum f_i N(a_i^\dagger a_i) + \frac{1}{4}\sum \Gamma_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k) + \frac{1}{36}\sum W_{ijklmn} N(a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l)$$

$$\begin{aligned}
E_{vac} &= \langle\Phi|H|\Phi\rangle \\
f_i &= t_{ii} + \sum_h \langle ih|V_2|ih\rangle\, n_h + \frac{1}{2}\sum_{hh'} \langle ihh'|V_3|ihh'\rangle\, n_h n_{h'} \\
\Gamma_{ijkl} &= \langle ij|V_2|kl\rangle + \sum_h \langle ijh|V_3|klh\rangle\, n_h \\
W_{ijklmn} &= \langle ijk|V_3|lmn\rangle
\end{aligned}$$

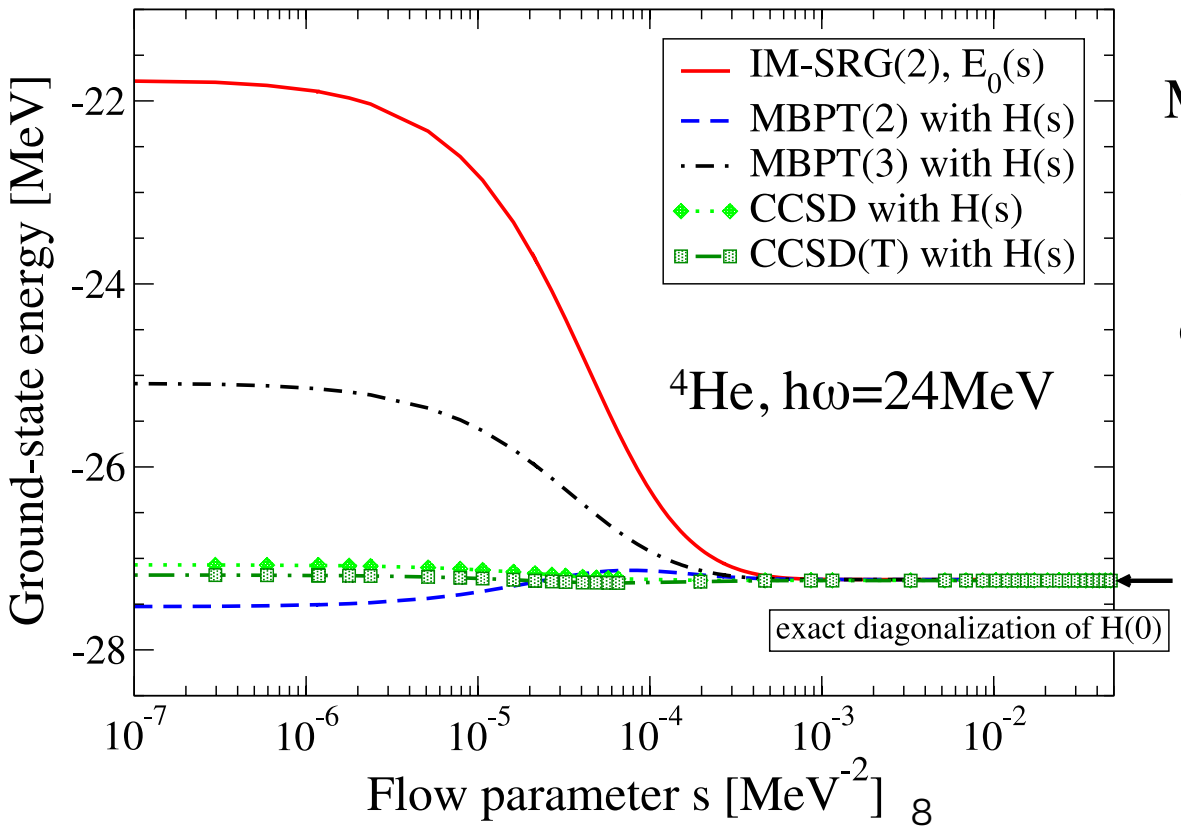
$$\langle\Phi|N(\cdots)|\Phi\rangle = 0$$

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N?



H^{od} gets suppressed.

Many-body methods w/evolved *H(s)*

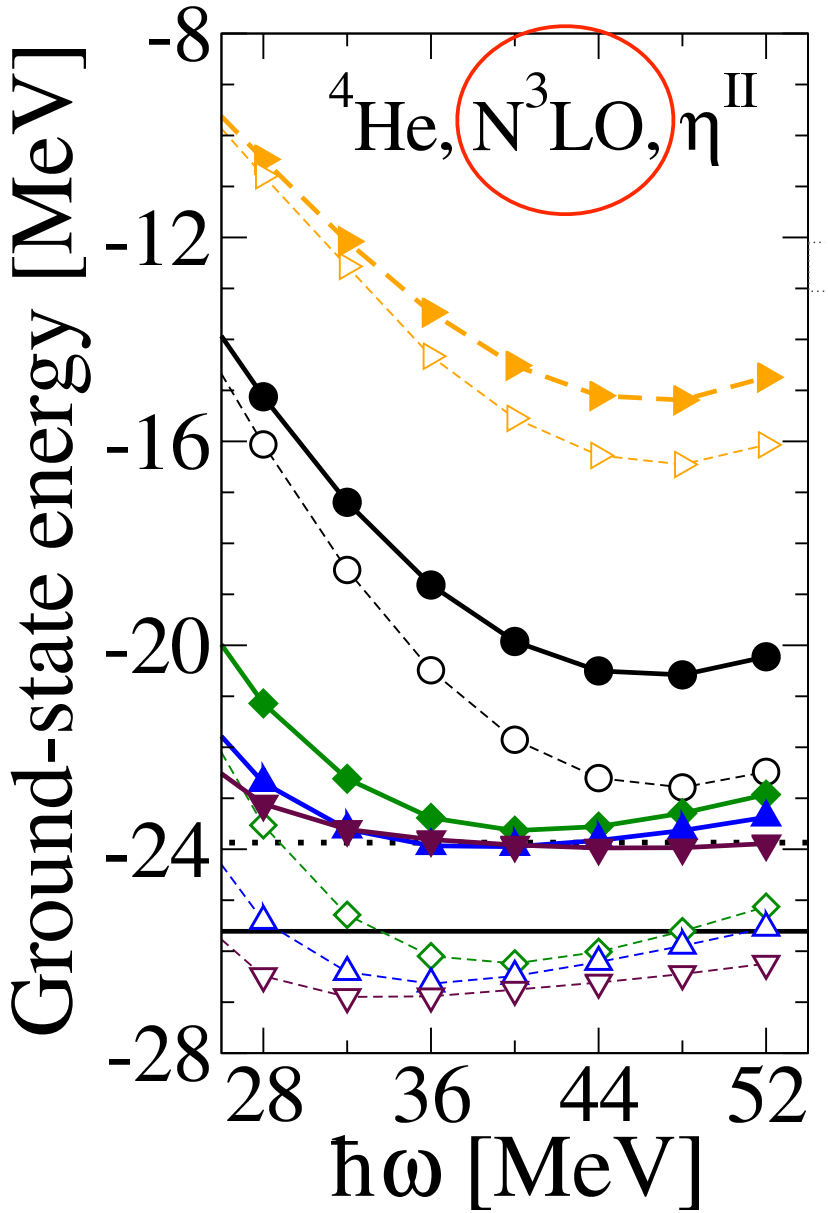


MBPT converges more quickly

S-independent CCSD(T)
=> IM-SRG(2) is controllable approximation.

$$\lambda \equiv s^{-1/4}$$

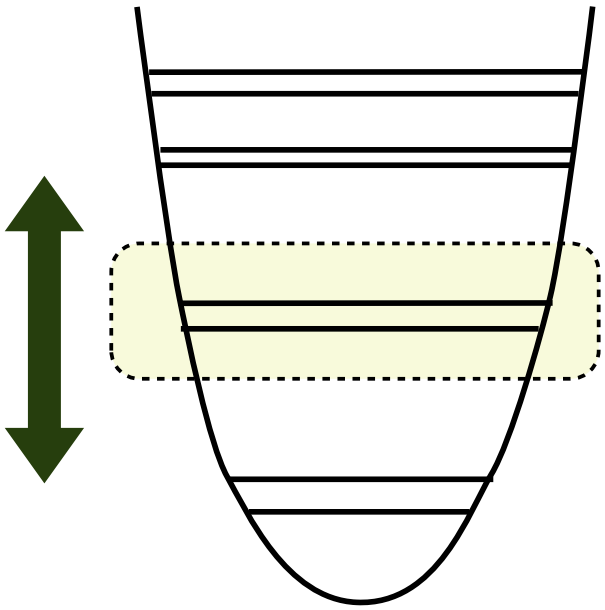
Dependence on truncation for harder interactions



Consistent IM-SRG(2)' truncation (solid) converges to CCSD result

Substantial overbinding in each emax space for naive original IM-SRG(2) truncation (open)

Shell model effective interactions from the IM-SRG



Passive valence orbitals $\{q_i\}$

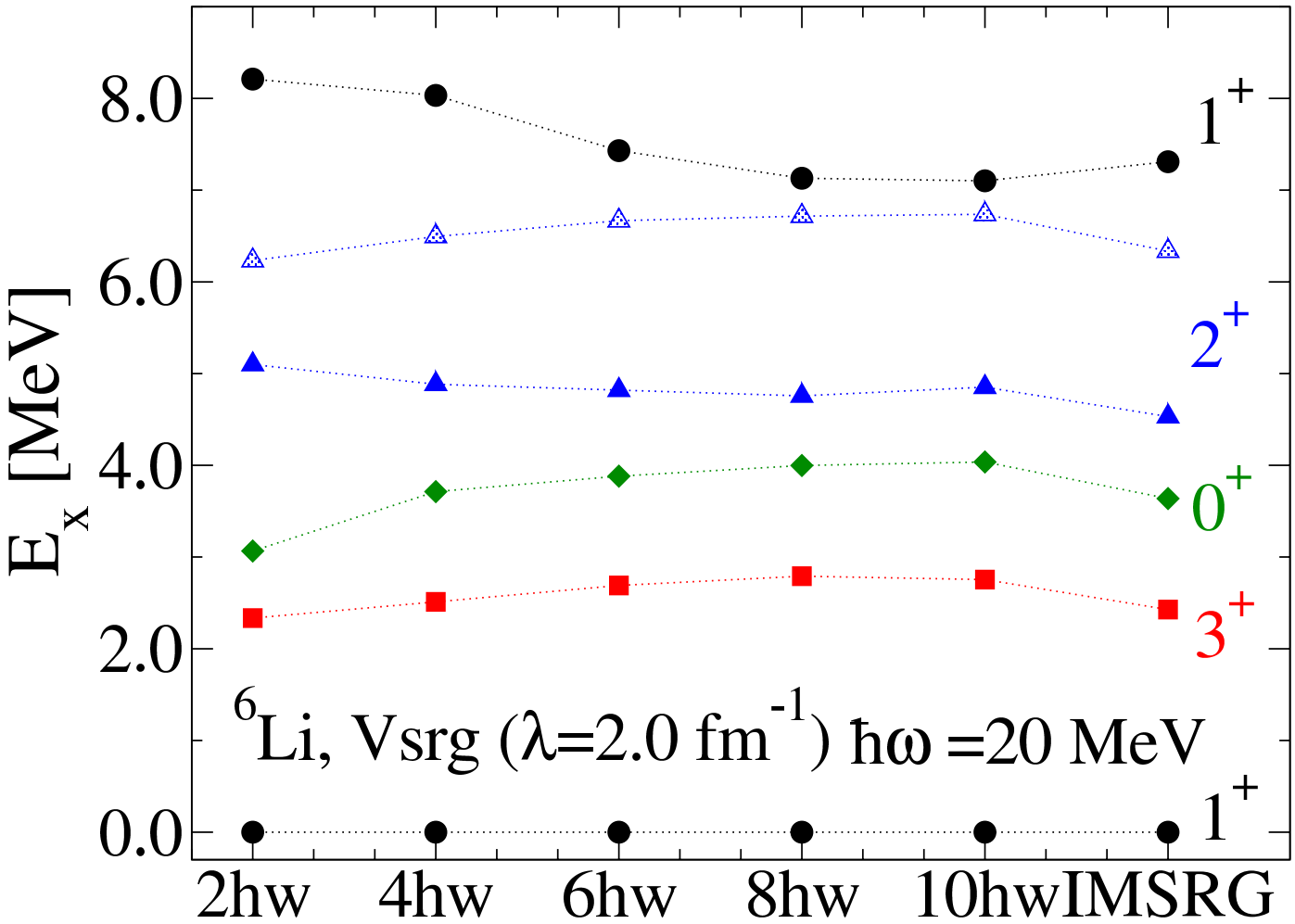
Active valence orbitals $\{v_i\}$

hole orbitals $\{h_i\}$

$$f^{\mathrm{od}}(s) = \sum_{ph} f_{ph}(s)\,\{a_p^\dagger a_h\} + \sum_{vq} f_{vq}(s)\,\{a_v^\dagger a_q\} + \sum_{vh} f_{vq}(s)\,\{a_v^\dagger a_h\}$$

$$\Gamma^{\mathrm{od}}(s) = \sum_{pp'hh'} \Gamma_{pp'hh'}(s)\,\{a_p^\dagger a_{p'}^\dagger a_{h'} a_h\} + \sum_{pp'vh} \Gamma_{pp'vh}\,\{a_v^\dagger a_{v'}^\dagger a_h a_p\}$$
$$+ \sum_{vv'qq'} \Gamma_{vv'qq'}(s)\,\{a_v^\dagger a_{v'}^\dagger a_{q'} a_q\} + \sum_{vv'v''q} \Gamma_{vv'v''q}\,\{a_v^\dagger a_{v'}^\dagger a_q a_{v''}\}$$

Excitation spectra of ^{6}Li versus NCSM result



Summary and Outlook

- ☑ IM-SRG for closed-shell nuclei
  - ☑ implemented other generators
  - ☑ consistent truncation worked out based on MBPT content
  - ☑ harder interactions (“bare” n3lo) treated
  - ☑ Contamination of center of mass excitation is very small.
  - ☑ comparable to CCSD in current truncation
  - ☑ tools in place for benchmark paper of medium-mass nuclei (w/CC, SCGF, UMOA)

- ☑ Shell-model effective interactions for valence nucleons.
  - ☑ proof of principle for 6Li carried out
  - ☑ seems to outperform traditional MBPT methods

Summary and Outlook

Work in Progress

- initial 3N (normal ordered 0,1,2-body parts)
- effective operator/Hamiltonian for open-shell systems.
  - Effective interaction for valence shell nucleons (p, sd, fp).
  - effective charge ==> B(E2) for C, Ca, Ni and Sn.
  - quenching factor for GT transition.
- Systematic improvement; 3-body flow equations (derived, not yet coded).
- particle-hole channels in infinite matter (H. Hergert)
- HFB reference state (H. Hergert)

Articles and Preprints Citing SCIDAC Support

✓ Published or Posted since MSU 2010

- "An improved density matrix expansion for spin-unsaturated nuclei," B. Gebremariam, T. Duguet, and S.K. Bogner, Phys. Rev. C **82**, 014305 (2010).
- "Natural units for nuclear energy density functional theory," M. Kortelainen, R.J. Furnstahl, W. Nazarewicz, and M.V. Stoitsov, Phys. Rev. C **82**, 011304(R) (2010).
- "Operator Evolution via the Similarity Renormalization Group I: The Deuteron," E.R. Anderson, S.K. Bogner, R.J. Furnstahl, and R.J. Perry, Phys. Rev. C **82**, 054001 (2010).
- "Microscopically-constrained Fock energy density functionals from chiral effective field theory. I. Two-nucleon interactions," B. Gebremariam, S.K. Bogner, and T. Duguet, Nucl. Phys. A **851**, 17 (2011).
- "In-medium similarity renormalization group for nuclei," K. Tsukiyama, S.K. Bogner, and A. Schwenk, Phys. Rev. Lett. 106, 222502 (2011).
- "Decoupling of Spurious Deep Bound States with the Similarity Renormalization Group," K.A. Wendt, R.J. Furnstahl, and R.J. Perry, Phys. Rev. C **83**, 034005 (2011).

Articles and Preprints Citing SCIDAC Support

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- "Evolving Nuclear Many-Body Forces with the Similarity Renormalization Group," E.D. Jurgenson, P. Navratil, and R.J. Furnstahl, Phys. Rev. C **83**, 034301 (2011).
- "Improved nuclear matter calculations from chiral low-momentum interactions," K. Hebeler, S.K. Bogner, R.J. Furnstahl, A. Nogga, and A. Schwenk, Phys. Rev. C **83**, 031301 (2011).
- "Chiral three-nucleon forces and pairing in nuclei," T. Lesinski, K. Hebeler, T. Duguet, and A. Schwenk, arXiv:1104.2955.
- "Quasiparticle Random Phase Approximation with Interactions from the Similarity Renormalization Group," H. Hergert, P. Papakonstantinou, and R. Roth, arXiv:1104.0264.
- "Exact-exchange density functional theory for neutron drops," J.E. Drut and L. Platter, arXiv:1104.4357.
- "The Similarity Renormalization Group with Novel Generators," W. Li, E.R. Anderson, R.J. Furnstahl, arXiv:1106.2835.
- "Testing the density matrix expansion against ab initio calculations of trapped neutron drops," S.K. Bogner, R.J. Furnstahl, H. Hergert, M. Kortelainen, P. Maris, M. Stoitsov, J.P. Vary, arXiv:1106.3557.

Ab Initio Functional Year-5 Deliverable Scoreboard

Plan for Year-5 from Continuation Progress Report

- ✓ Develop and test improved DME functionals that go beyond HF ( microscopic pairing; constrain volume terms from BHF).
- ✓ Perform neutron drop benchmarks starting from NN and  NNN interactions and validate against ab-initio calculations.
- Develop the Optimized Effective Potential (OEP) method for  3D-HFB; compare with ✓ HF, HF-DME, and ab initio.
- Use ✓ in-medium SRG to develop  valence shell model Hamiltonians and effective operators for open-shell nuclei.

Other deliverables from CPR

- Compare DME to  CC and ✓ NCFC with the same (variable) Hamiltonian, including with external fields.
- ✓ Improve and test infinite matter on which DME relies;  initial steps toward Monte Carlo and CC calculations
- ✓ Apply $NN + NNN$ low-k SRG interactions in p-shell with NCFC
- SRG: ✓ develop few-body operators, test factorization, ✓ explore alternative generators to control many-body operators