Applications of Renormalization Group Methods in Nuclear Physics – 5

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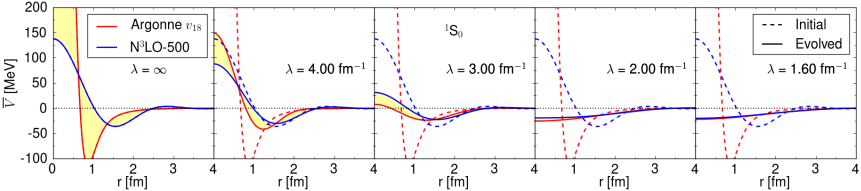
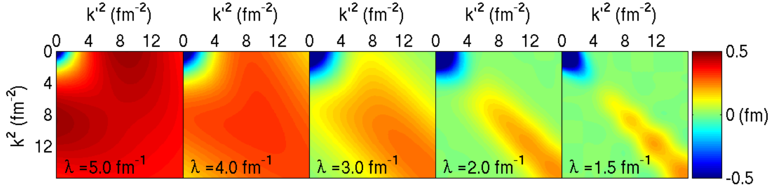
HUGS 2014





Outline: Lecture 5

Lecture 5: New methods and IM-SRG in detail

- New methods with some applications
- In-Medium Similarity Renormalization Group

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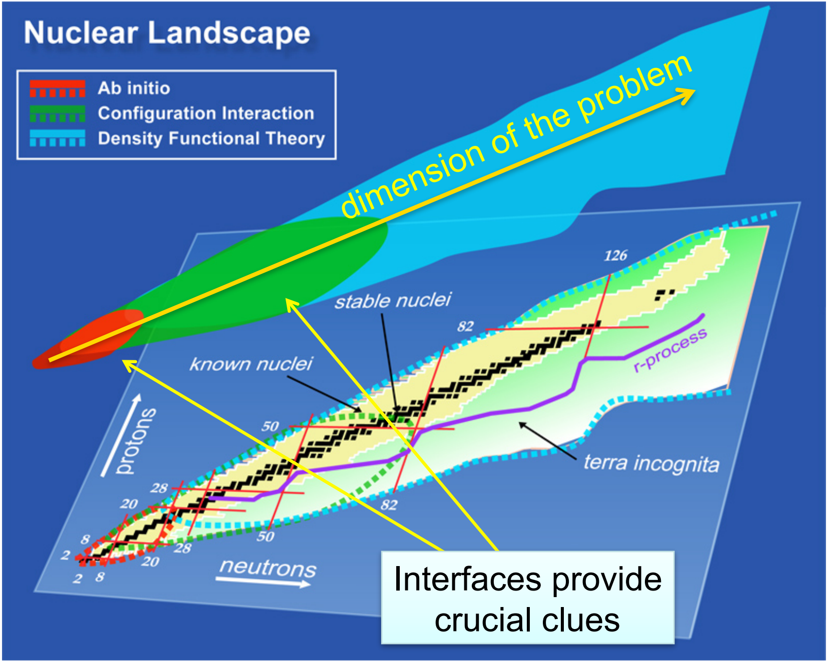
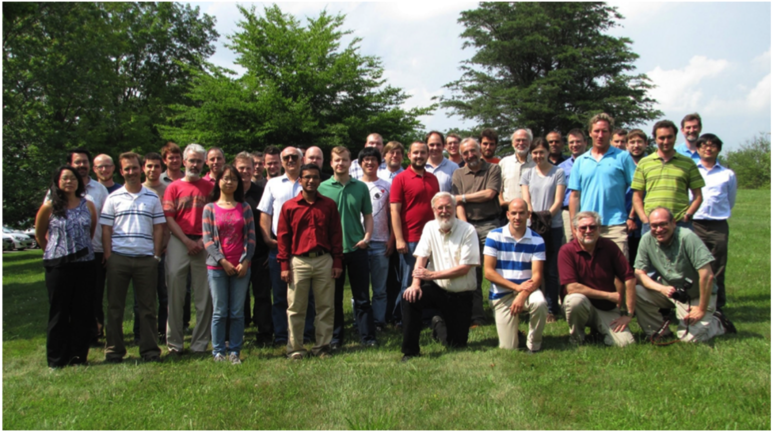
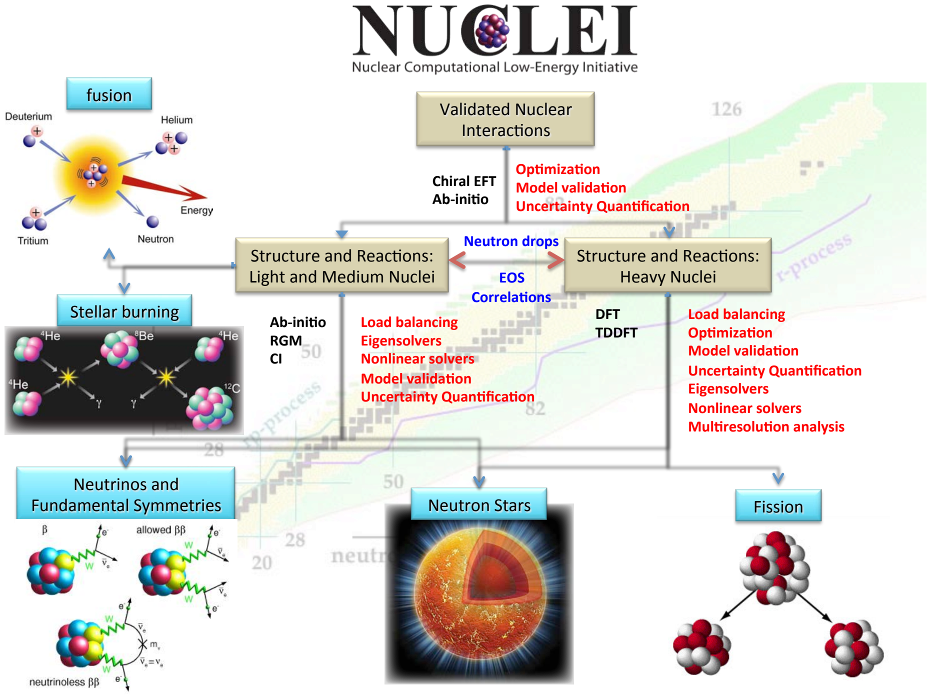

Nuclear Landscape
Ab initio
Configuration Interaction
Density Functional Theory
dimension of the problem
stable nuclei
known nuclei
126
82
50
28
20
8
2
r-process
terra incognita
protons
neutrons
Interfaces provide crucial clues

SciDAC-2 NUCLEI Project

- NUclear Computational Low Energy Initiative
- Collaboration of physicists, applied mathematicians, and computer scientists $\Longrightarrow$ builds on UNEDF project [unedf.org]
- US funding but many international collaborators
- See computingnuclei.org for highlights!




NUCLEI
Nuclear Computational Low-Energy Initiative
fusion
Deuterium
Helium
Energy
Tritium
Neutron
Validated Nuclear Interactions
Chiral EFT
Ab-initio
Optimization
Model validation
Uncertainty Quantification
Structure and Reactions: Light and Medium Nuclei
Neutron drops
EOS
Correlations
Structure and Reactions: Heavy Nuclei
Stellar burning
4He
8Be
4He
4He
12C
γ
γ
Ab-initio
RGM
CI
Load balancing
Eigensolvers
Nonlinear solvers
Model validation
Uncertainty Quantification
DFT
TDDFT
Load balancing
Optimization
Model validation
Uncertainty Quantification
Eigensolvers
Nonlinear solvers
Multiresolution analysis
Neutrinos and Fundamental Symmetries
β
allowed ββ
neutrinoless ββ
Neutron Stars
Fission
126
82
50
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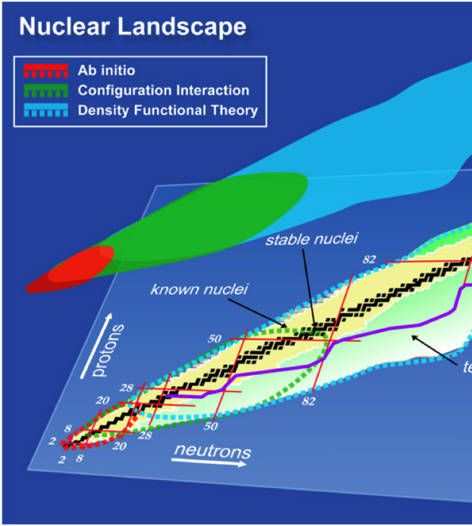
20
r-process
rp-process

Explosion of many-body methods using microscopic input

- Ab initio (new and enhanced methods; microscopic NN+3NF)
  - Stochastic: GFMC/AFDMC (new: with local EFT); lattice EFT
  - Diagonalization: IT-NCSM
  - Coupled cluster (CCSD(T), CR-CC(2,3), Bogoliubov, . . .)
  - IM-SRG (In-medium similarity renormalization group)
  - Self-consistent Green's function
  - Many-body perturbation theory
- Shell model (usual: empirical inputs)
  - Effective interactions from coupled cluster, IM-SRG
- Density functional theory
  - Microscopic input, e.g., through density matrix expansion



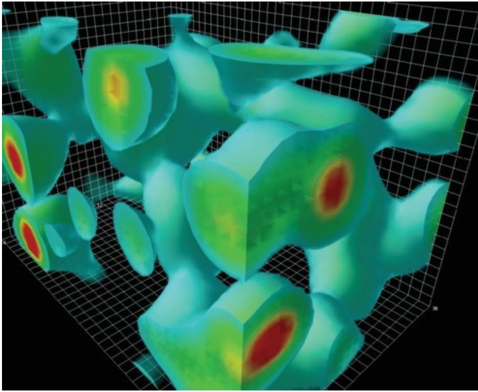
Do we really need all of these methods?

Compare to lattice QCD: Are all the different lattice actions needed?

- clover quarks on anisotropic lattices (mass spectrum)
- domain wall quarks (chiral symmetry)
- highly improved staggered quarks (high-precision extrapolations)
- and more!

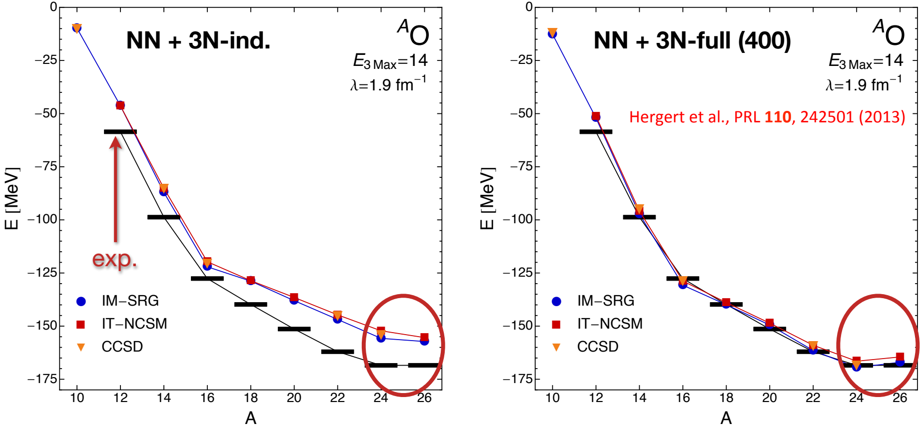
Answer: yes!

- Complementary strengths
- Cross-check results
- Identify theory error bars



A frame from an animation illustrating the typical four-dimensional structure of gluon-field configurations used in describing the vacuum properties of QCD.

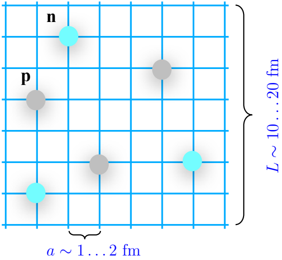
Oxygen chain with 3 methods [from H. Hergert et al. (2013)]

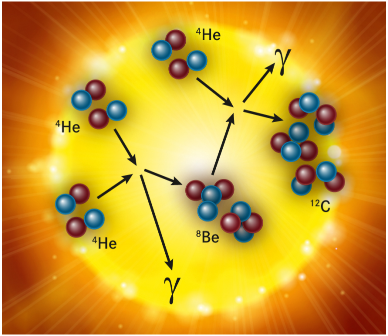


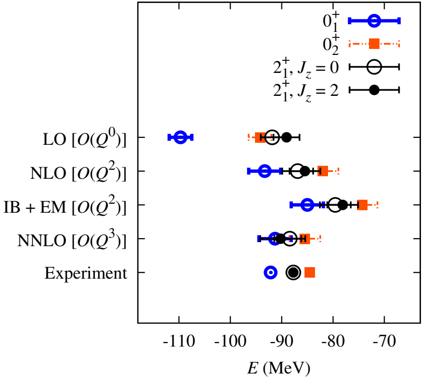
- In-medium SRG, importance-truncated NCSM, coupled cluster
- Same Hamiltonian $\Longrightarrow$ test for consistency between *methods*
- Impact of three-nucleon force (3NF) on dripline
- Need precision experiment *and* theory

Hoyle state from lattice chiral EFT [E. Epelbaum et al.]

- Triple-α resonance in ^{12}C
- Low-resolution (coarse) lattice
- Suited to adjust to clusters
- Order-by-order improvement: LO $\Longrightarrow$ NLO $\Longrightarrow$ N^{2}LO
- [Also high-precision GFMC!]







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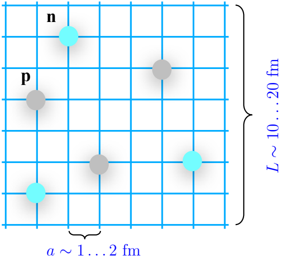
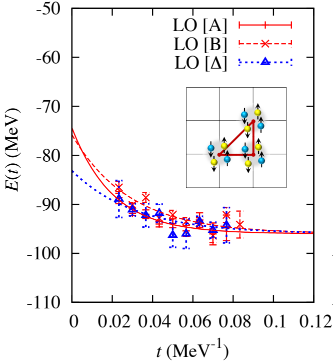
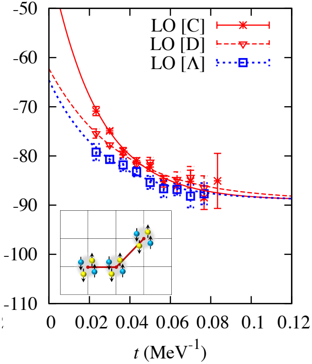




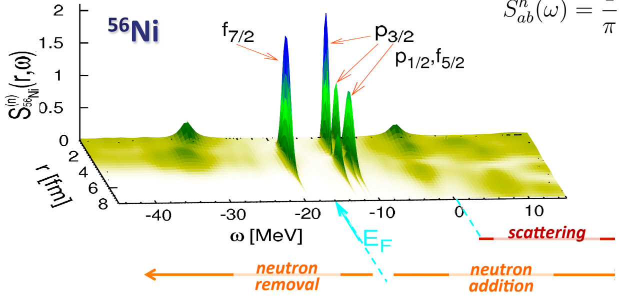


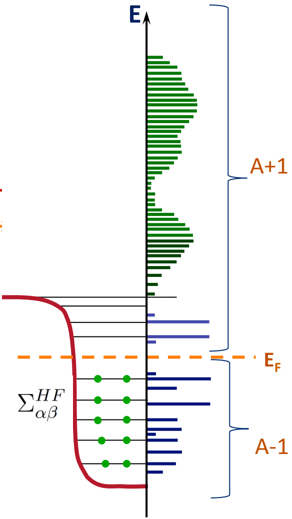
- Probing α cluster structure of 0^+ states
- How does the triple-α reaction rate depend on the quark mass?
- Much more!
- Most recent: ^{16}O structure

Spectral functions from self-consistent Green's function

[figures from C. Barbieri]

$$S^h_{ab}(\omega) = \frac{1}{\pi}\, Im\, g_{ab}(\omega)$$

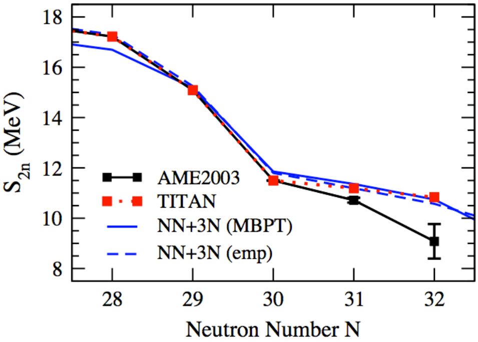


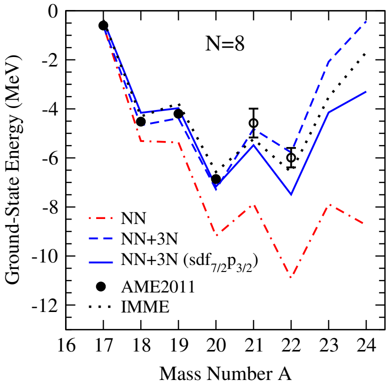


- One-body Greens function (or propagator) $g_{ab}(\omega)$ describes the motion of quasi-particles and quasi-holes
- Contains all the structure information probed by nucleon transfer
- Imaginary (absorptive) part of $g_{ab}(\omega)$ is the spectral function

Confronting theory and experiment to both driplines

- Precision mass measurements test impact of chiral 3NF
- Proton rich [Holt et al. (2012)]
- Neutron rich [Gallant et al. (2012)]
- Many new tests possible!





- Shell model description using chiral potential evolved to $V_{\text{low }k}$ plus 3NF fit to $A = 3, 4$
- Excitations outside valence space included in 3rd order MBPT

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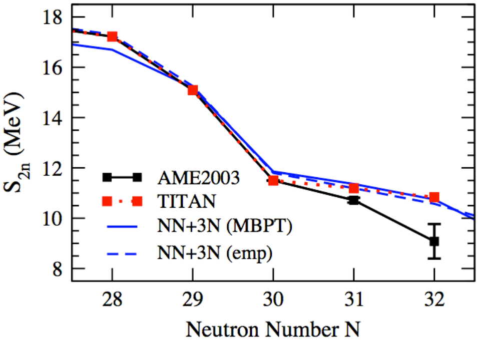

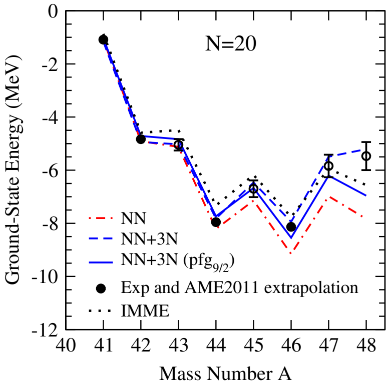

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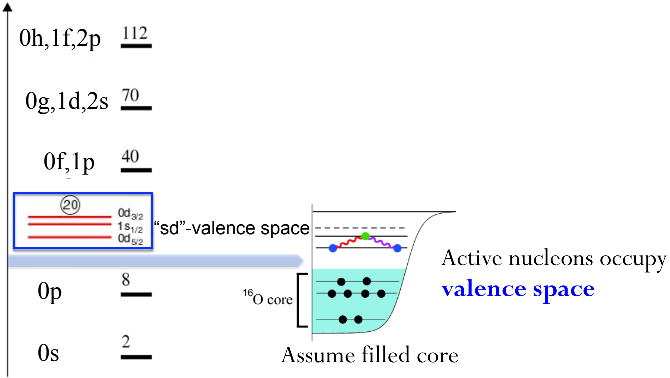
Non-empirical shell model [from J. Holt]

Solving the Nuclear Many-Body Problem

Nuclei understood as many-body system starting from closed shell, add nucleons

Interaction and energies of valence space orbitals from original $V_{\text{low }k}$

This alone does not reproduce experimental data



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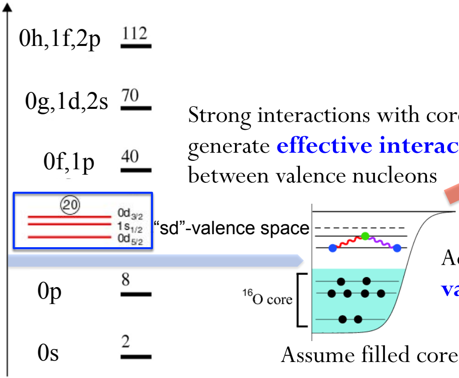
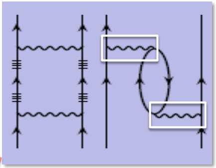


Strong interactions with core generate **effective interaction** between valence nucleons

Hjorth-Jensen, Kuo, Osnes (1995)



Active nucleons occupy **valence space**

Assume filled core

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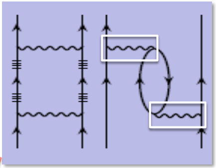
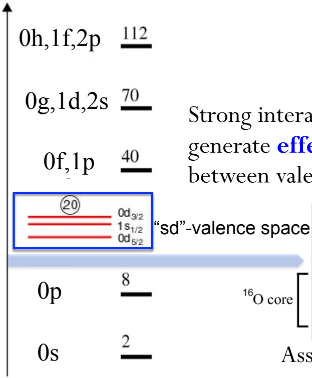
Effective two-body matrix elements

Single-particle energies (SPEs)

Hjorth-Jensen, Kuo, Osnes (1995)





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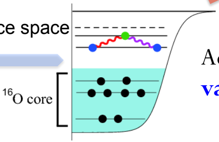


Active nucleons occupy **valence space**

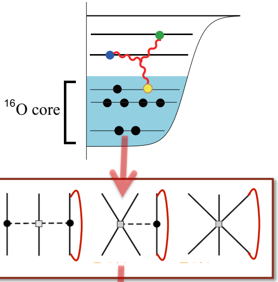
Assume filled core

Chiral 3NFs meet the shell model [from J. Holt]

3N Forces for Valence-Shell Theories

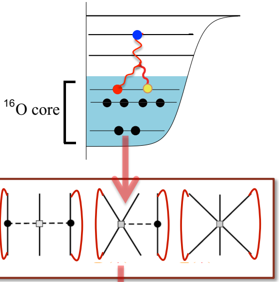
Normal-ordered 3N: contribution to valence neutron interactions

Effective two-body



$$\langle ab|\, V_{3N,\mathrm{eff}} \,|a'b'\rangle = \sum_{\alpha=core} \langle \alpha ab|\, V_{3N} \,|\alpha a'b'\rangle$$

Effective one-body



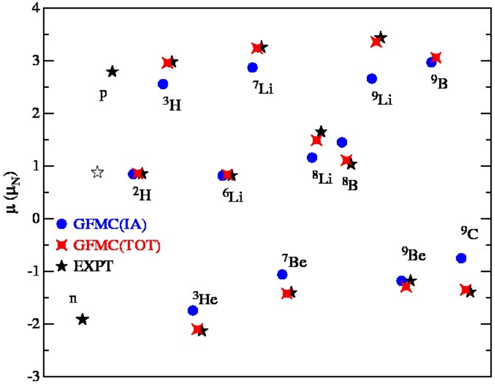
$$\langle a|\, V_{3N,\mathrm{eff}} \,|a'\rangle = \frac{1}{2} \sum_{\alpha\beta=core} \langle \alpha\beta a|\, V_{3N} \,|\alpha\beta a'\rangle$$

Combine with microscopic NN: eliminate empirical adjustments

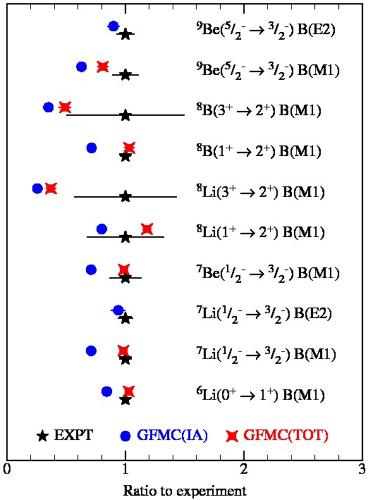
GFMC: Calculating observables in light nuclei

- Green's Function Monte Carlo (GFMC) energies are accurate but lowest-order theory of one-body currents (blue) disagrees with experiment (black)
- Including two-nucleon currents based on EFT (red) improves all predictions!

Magnetic Moments



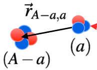
Electromagnetic Transitions



Note: not fully consistent yet!

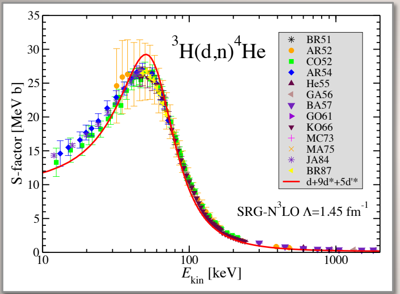
Combining structure and reactions [P. Navratil et al.]

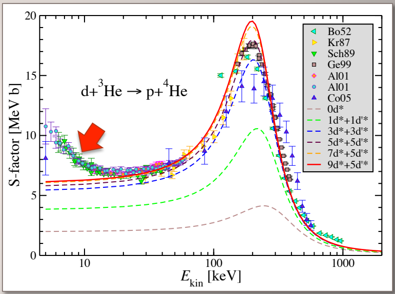
Resonating Group Method + NCSM:



$\psi_{1\nu}^{(A-a)}\psi_{2\nu}^{(a)}\delta(\vec{r}-\vec{r}_{A-a,a})$

- NCSM/RGM with *SRG-N³LO NN* potentials





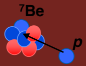
Potential to address unresolved fusion research related questions:
^{3}H(d,n)^{4}He fusion with polarized deuterium and/or tritium,
^{3}H(d,$n\,\gamma$)^{4}He bremsstrahlung,
Electron screening at very low energies …

P.N., S. Quaglioni, PRL **108**, 042503 (2012)

- Ab initio fusion! In progress: SRG-evolved NNN interactions

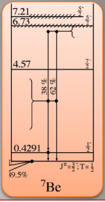
Combining structure and reactions [P. Navratil et al.]

TRIUMF



^{7}Be(p,γ)^{8}B radiative capture

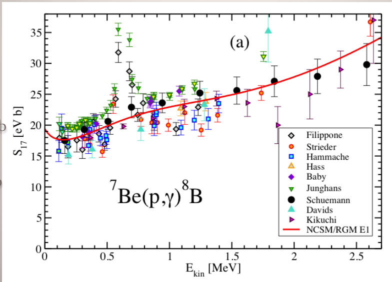
- NCSM/RGM calculation of ^{7}Be(p,γ)^{8}B radiative capture
  - ^{7}Be states $3/2^-$, $1/2^-$, $7/2^-$, $5/2^-_1$, $5/2^-_2$
  - Soft NN potential (SRG-N^{3}LO with Λ = 1.86 fm^{-1})

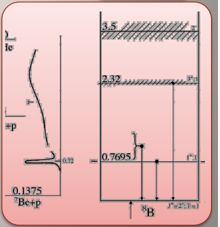


^{8}B 2$^+$ g.s. **bound** by 136 keV (expt. 137 keV)

S(0) ~ 19.4(0.7) eV b

Data evaluation: S(0)=20.8(2.1) eV b





The first ever *ab initio* calculations of ^{7}Be(p,γ)^{8}B

arXiv:1105.5977 [nucl-th]

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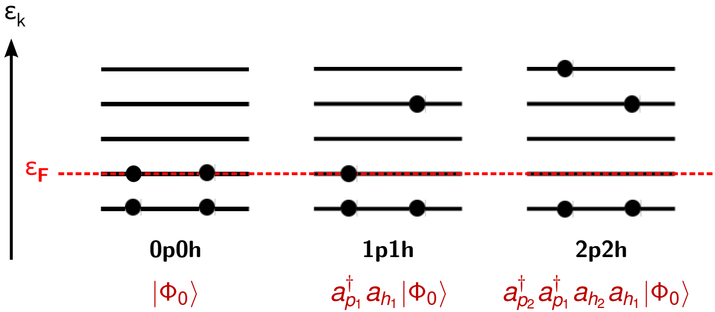
Lecture 5: New methods and IM-SRG in detail

- New methods with some applications
- In-Medium Similarity Renormalization Group

Choose a basis and a reference state $|\Phi_0\rangle$

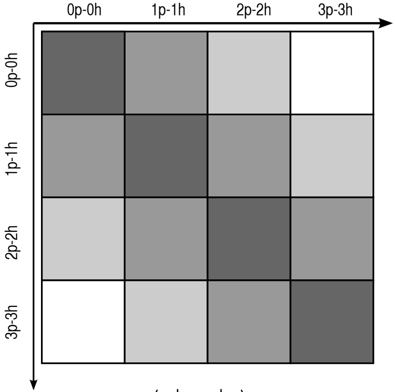
- The basis could be harmonic oscillators or Hartree-Fock or ...
- Anti-symmetric wave functions: A-particle Slater determinants
- Use second-quantization formalism: creation/destruction operators



- The reference state is filled, so no particles or holes: 0p–0h
- If one particle moved to a higher level, leaves hole behind: 1p–1h
- Complete basis: Slater determinants from all 1p–1h, 2p–2h, ...

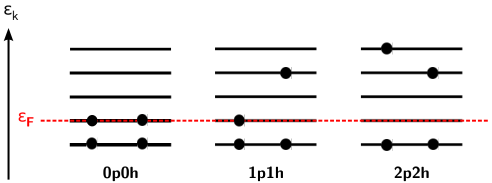
In-medium SRG decoupling [slides from H. Hergert]

Consider SRG with $0p$–$0h$ reference state (instead of vacuum)



$$\langle i | H | j \rangle$$

- Off-diagonal coupling between reference state and 1p–1h, 2p–2h basis states



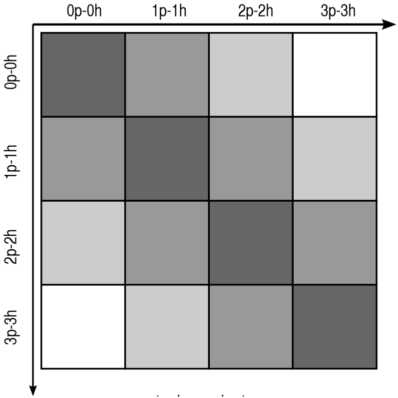
- Energy calculation requires full basis

K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL **106**, 222502 (2011)

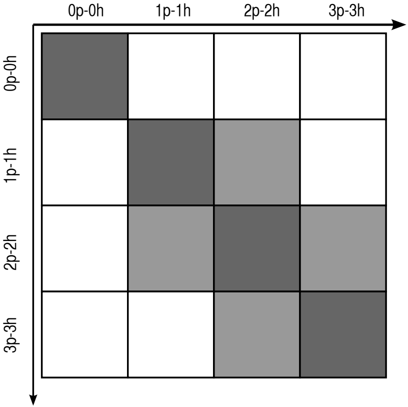
In-medium SRG decoupling [slides from H. Hergert]

IM-SRG: decouples reference state ($0p$–$0h$) from excitations

$\Longrightarrow$ Resummation of correlations into zeroth order E_0!



$\Longrightarrow$



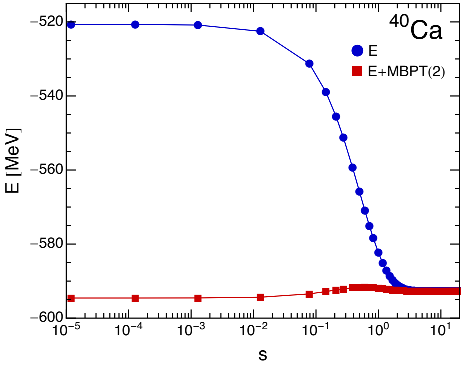
K. Tsukiyama, S. K. Bogner, and A. Schwenk, PRL **106**, 222502 (2011)

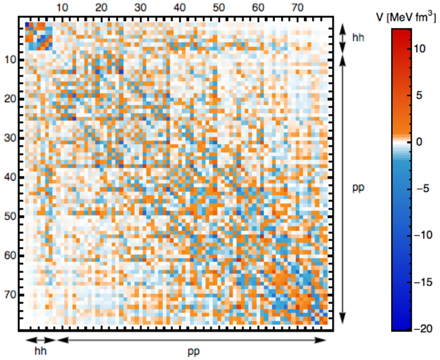
A new ab-initio structure method that can be applied directly *and* to generate shell-model effective interactions!

IM-SRG decoupling for ^{40}Ca [slides from H. Hergert]

IM-SRG: decouples reference state ($0p$–$0h$) from excitations

$\Longrightarrow$ Resummation of MBPT correlations into zeroth order E_0!





$V_{\mathrm{SRG}}(\mathrm{N3LO}), \lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

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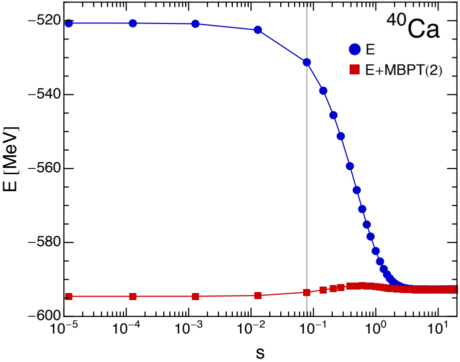

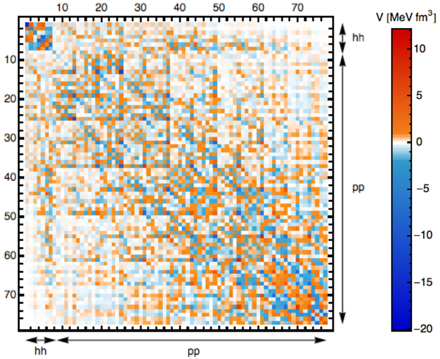

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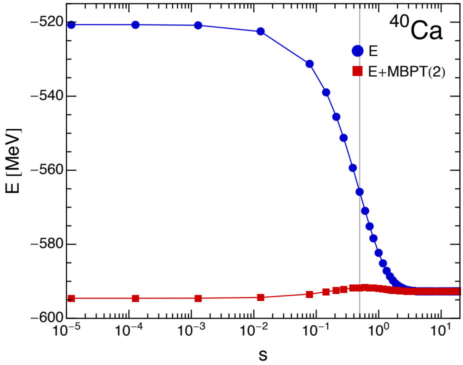

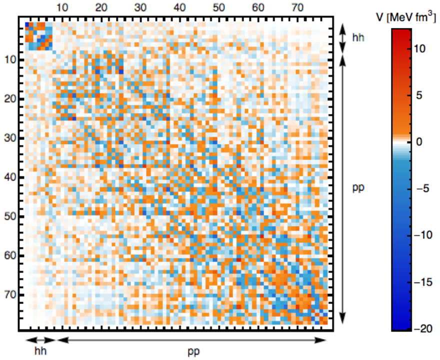

$V_{\mathrm{SRG}}(\mathrm{N3LO}), \lambda = 2.0\ \mathrm{fm}^{-1}, e_{\mathrm{Max}} = 8$

IM-SRG decoupling for ^{40}Ca [slides from H. Hergert]

IM-SRG: decouples reference state ($0p$–$0h$) from excitations

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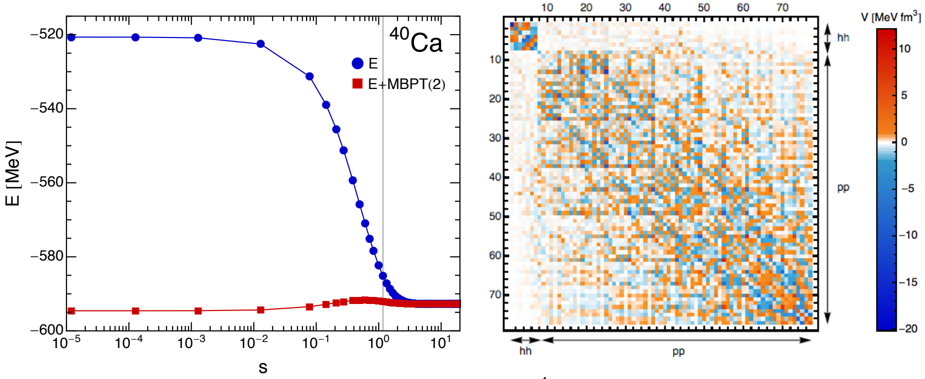

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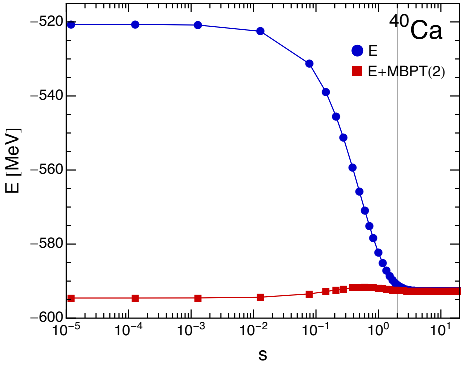

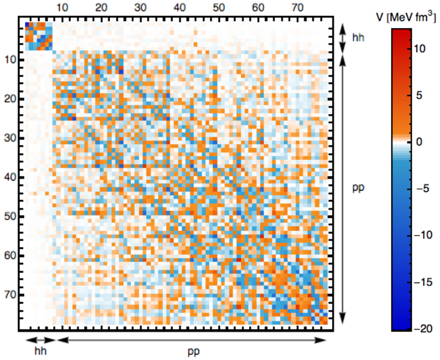

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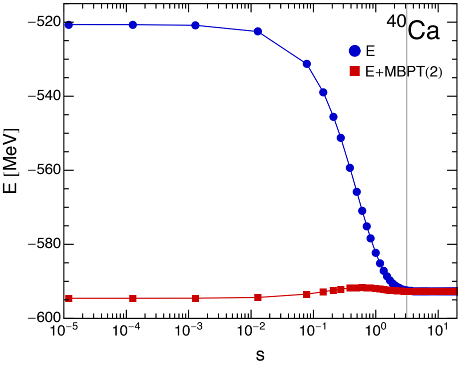

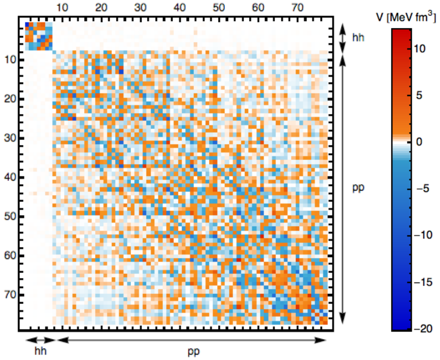

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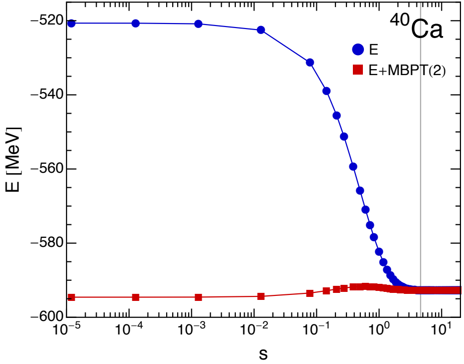

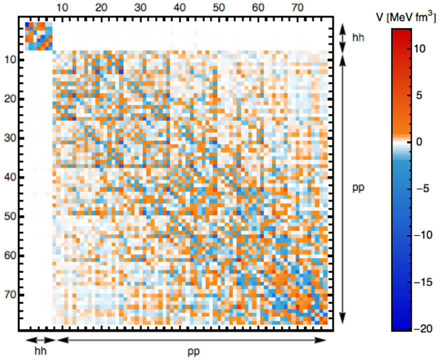

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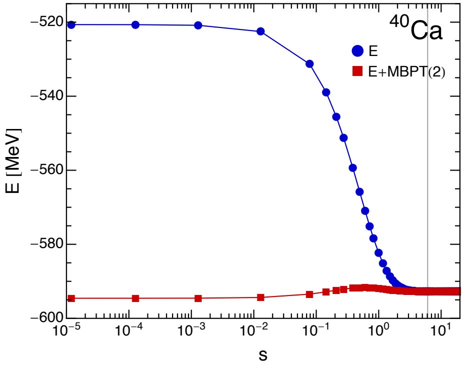

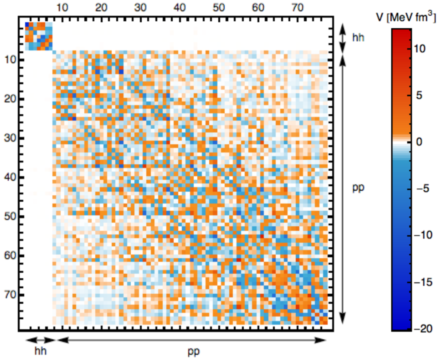

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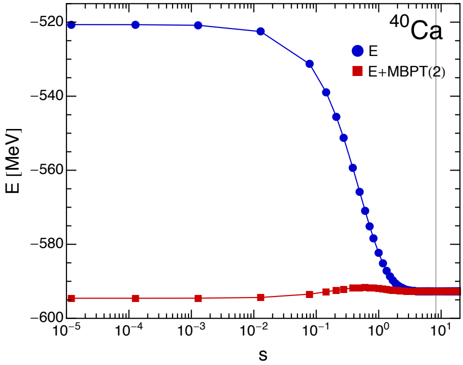
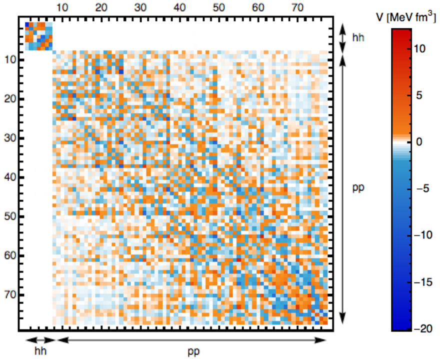


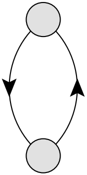


$V_{\text{SRG}}(\text{N3LO}), \lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

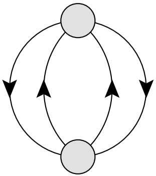
IM-SRG equations: Flow equations

0-body Flow

$$\frac{dE}{ds} =$$



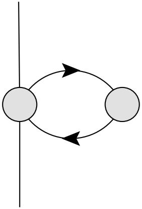
$$+$$



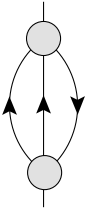
1-body Flow

$$\frac{df}{ds} =$$

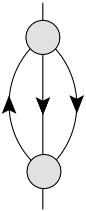
$$+$$



$$+$$

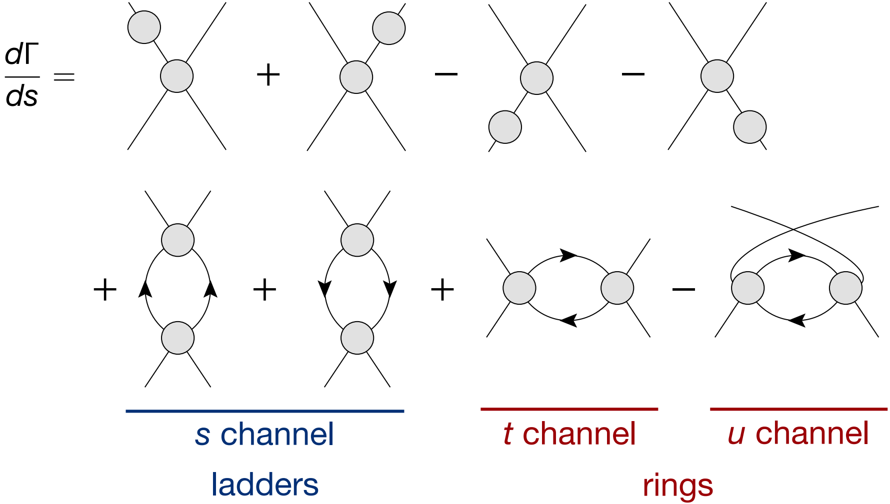


$$+$$



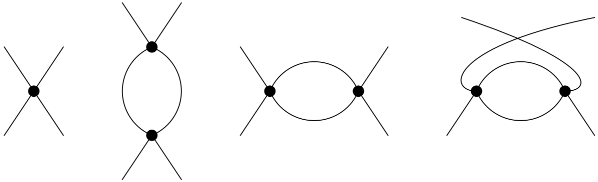
IM-SRG equations: Flow equation

2-body Flow

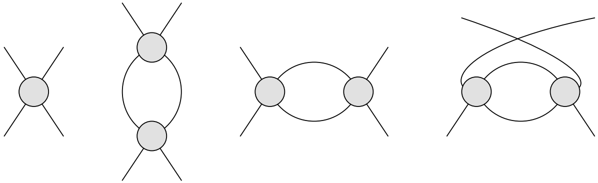


IM-SRG iteration: Nonperturbative resummation of MBPT

$\Gamma(\delta s) \sim$



$\Gamma(2\delta s) \sim$



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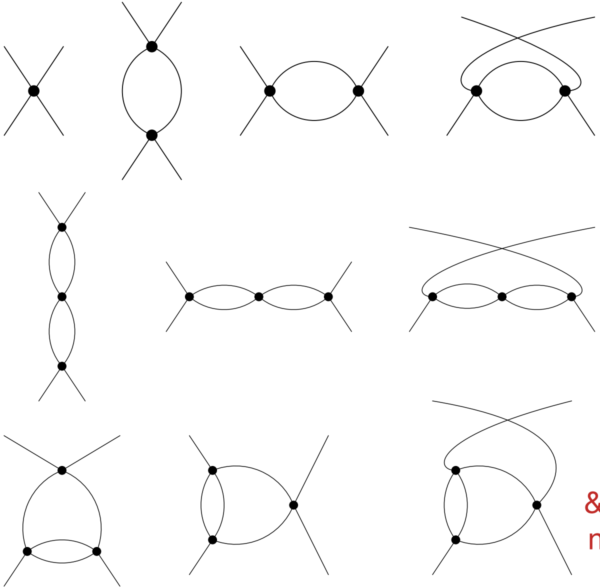
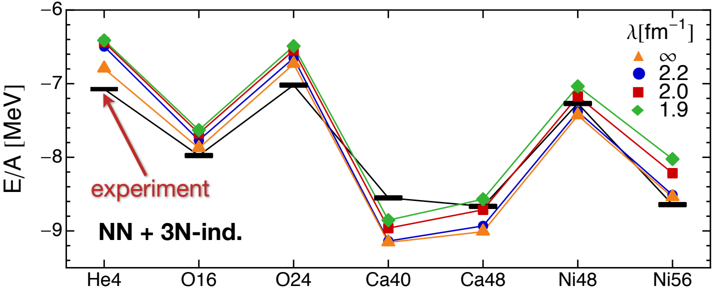


& many more...

IM-SRG results for closed-shell nuclei [slides from H. Hergert]



Phys. Rev. C **87**, 034307 (2013), arXiv: 1212.1190 [nucl-th]

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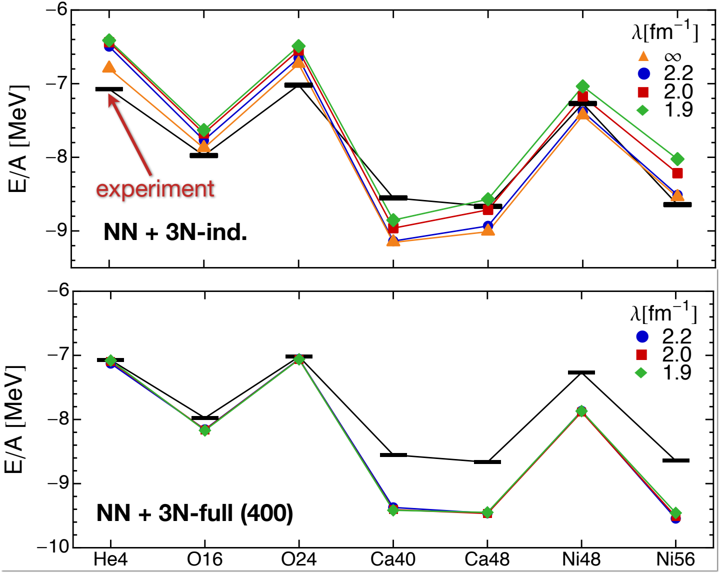

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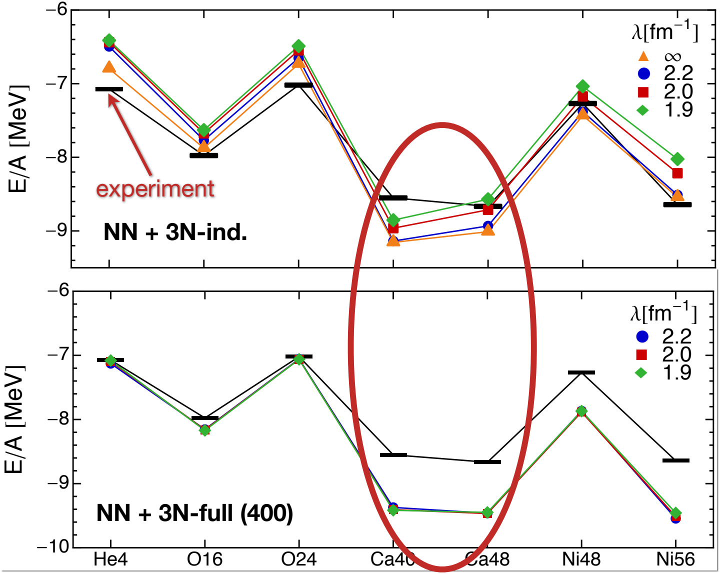

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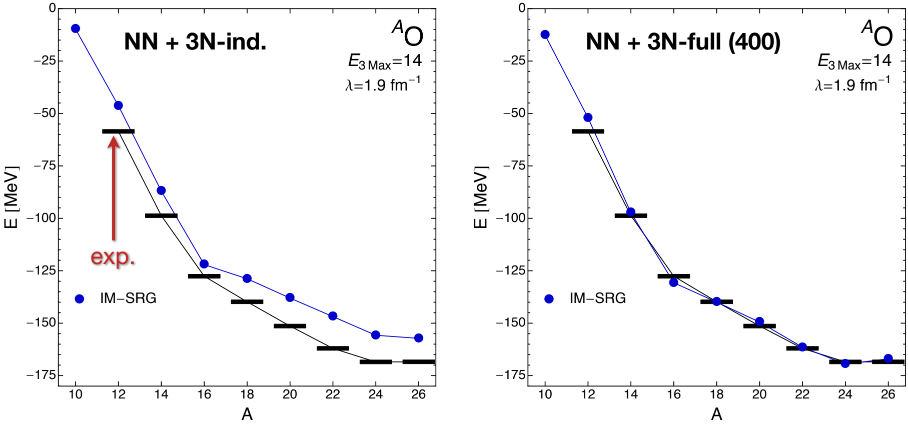
Multi-reference IM-SRG results for Oxygen chains

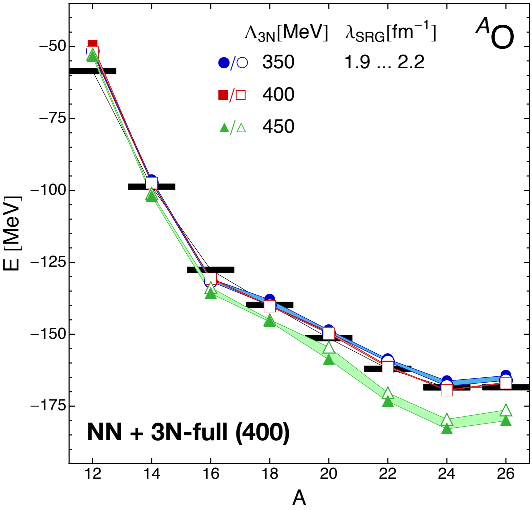
- Reference state: number-projected Hartree-Fock-Bogoliubov vacuum (pairing correlations)



Phys. Rev. Lett. **110**, 242501 (2013)

Multi-reference IM-SRG results for Oxygen chains

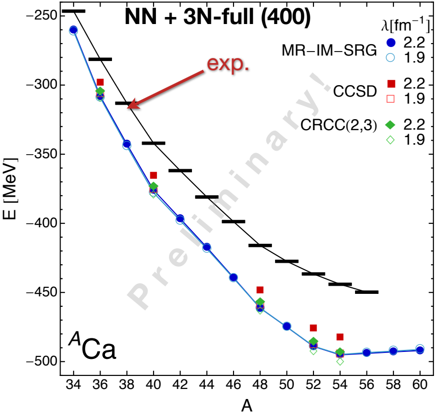
- Variation of initial 3N cutoff only
- Diagnostics for chiral EFT interactions
- Dripline at $A = 24$ is robust under variations

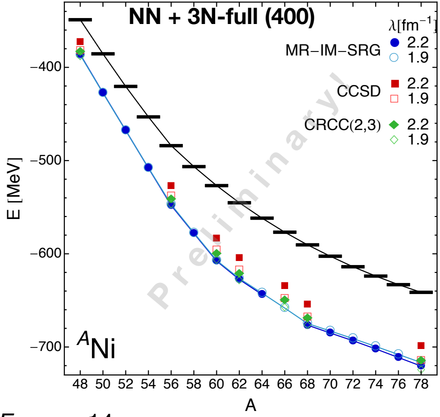


Phys. Rev. Lett. **110**, 242501 (2013)

IM-SRG results for Calcium and Nickel chains [preliminary]

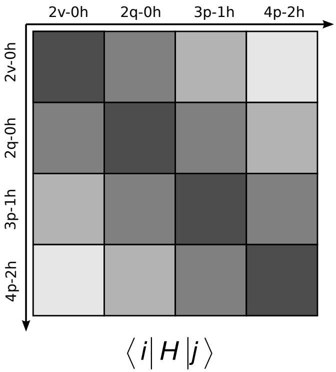
- Reference state: number-projected Hartree-Fock-Bogoliubov vacuum (pairing correlations)

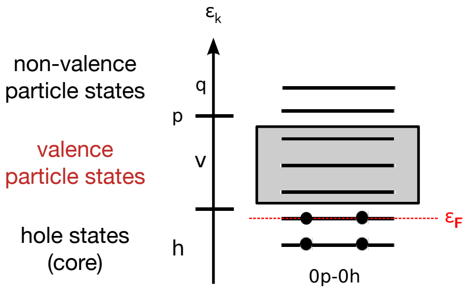




$e_{\mathrm{Max}} = 14,\ E_{3\mathrm{Max}} = 14$

IM-SRG valence-space decoupling [slides from H. Hergert]





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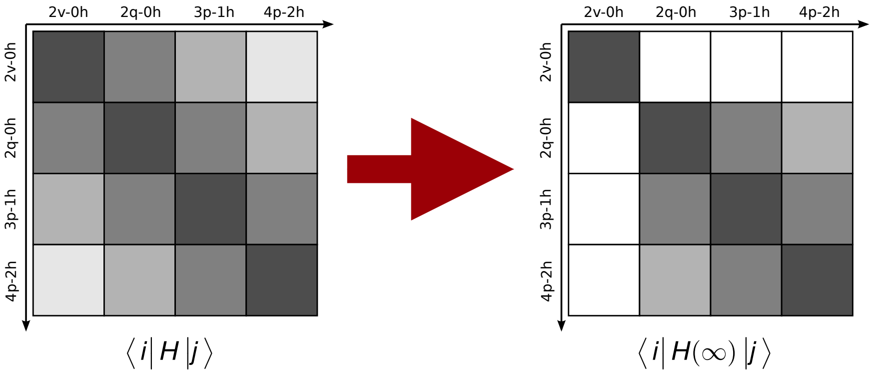
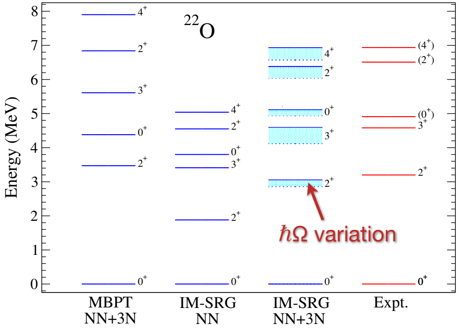
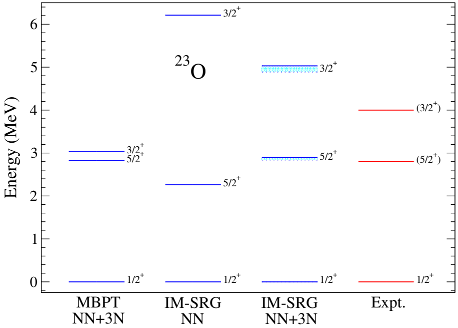


IM-SRG shell-model effective interaction [slides from H. Hergert]

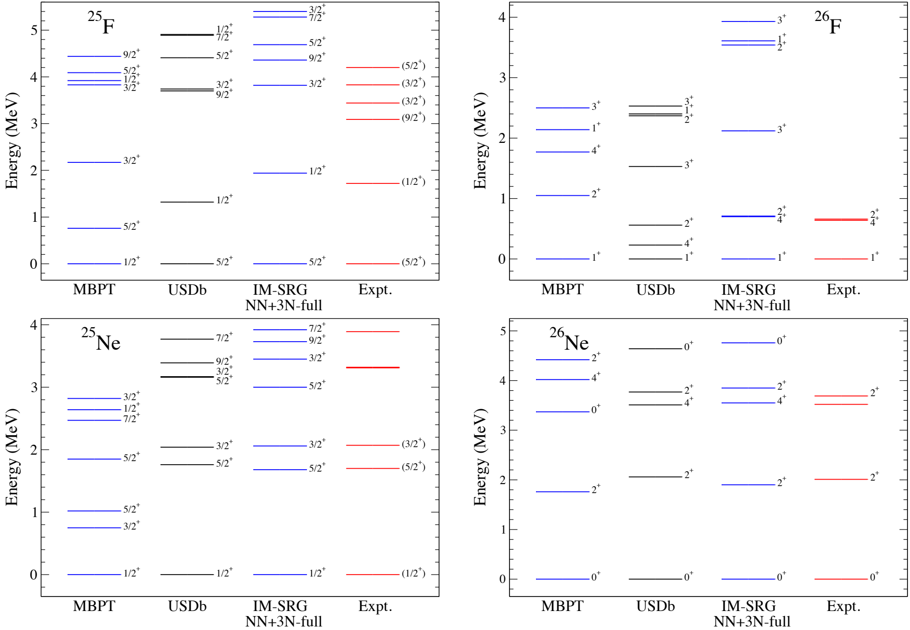




arXiv: 1402.1407 [nucl-th], [figures by J. Holt]

- 3N forces crucial
- IM-SRG improves on finite-order MBPT effective interaction
- Competitive with phenomenological calculations

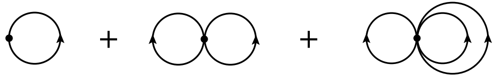
IM-SRG shell-model effective interaction [preliminary!]

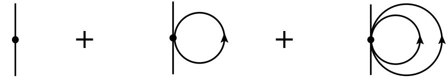


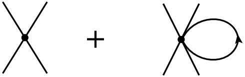
IM-SRG normal ordering [slides from H. Hergert]

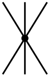
Normal-Ordered Hamiltonian

$$H = E_0 + \sum_{kl} f^k_l : A^k_l : + \frac{1}{4} \sum_{klmn} \Gamma^{kl}_{mn} : A^{kl}_{mn} : + \frac{1}{36} \sum_{ijklmn} W^{ijk}_{lmn} : A^{ijk}_{lmn} :$$

$E_0 =$ 

$f =$ 

$\Gamma =$ 

$W =$ 

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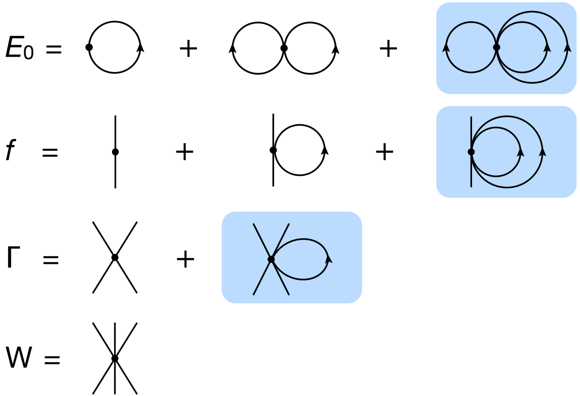

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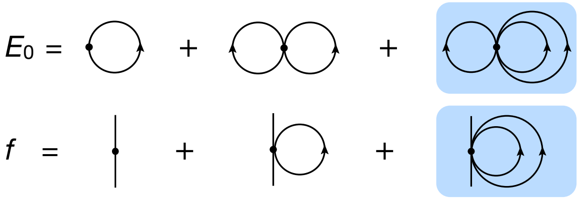

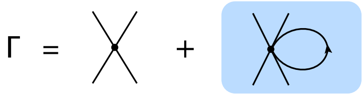

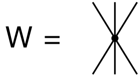

two-body formalism with in-medium contributions from three-body interactions

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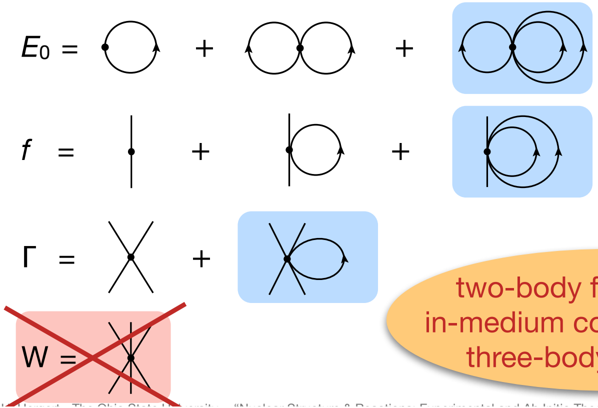
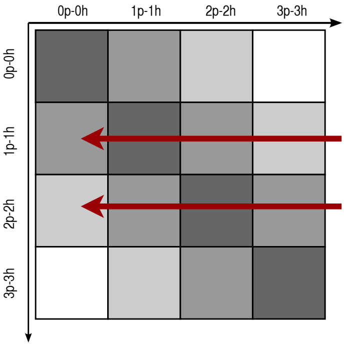


two-body formalism with in-medium contributions from three-body interactions

IM-SRG equations: Choice of generator



$$\left\langle {}^{p}_{h} \middle| H \middle| \Psi \right\rangle = \sum_{kl} f^{k}_{l} \left\langle \Psi \right| :A^{h}_{p} :: A^{k}_{l}: \left| \Psi \right\rangle = -n_h \bar{n}_p f^{p}_{h}$$

$$\left\langle {}^{pp'}_{hh'} \middle| H \middle| \Psi \right\rangle = \sum_{klmn} \Gamma^{kl}_{mn} \left\langle \Psi \right| :A^{hh'}_{pp'} :: A^{kl}_{mn}: \left| \Psi \right\rangle \sim \Gamma^{pp'}_{hh'}$$

Off-Diagonal Hamiltonian & Generator

$$H^{od} \equiv f^{od} + \Gamma^{od}\,, \quad f^{od} \equiv \sum_{ph} f^{p}_{h} :A^{p}_{h}: + \text{H.c.}\,, \quad \Gamma^{od} \equiv \sum_{pp'hh'} \Gamma^{pp'}_{hh'} :A^{pp'}_{hh'}: + \text{H.c.}$$