In-medium SRG for Nuclei

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PHYSICAL REVIEW C VOLUME 7, NUMBER 5 MAY 1973

Convergence Rate of Intermediate-State Summations in the Effective Shell-Model Interaction*

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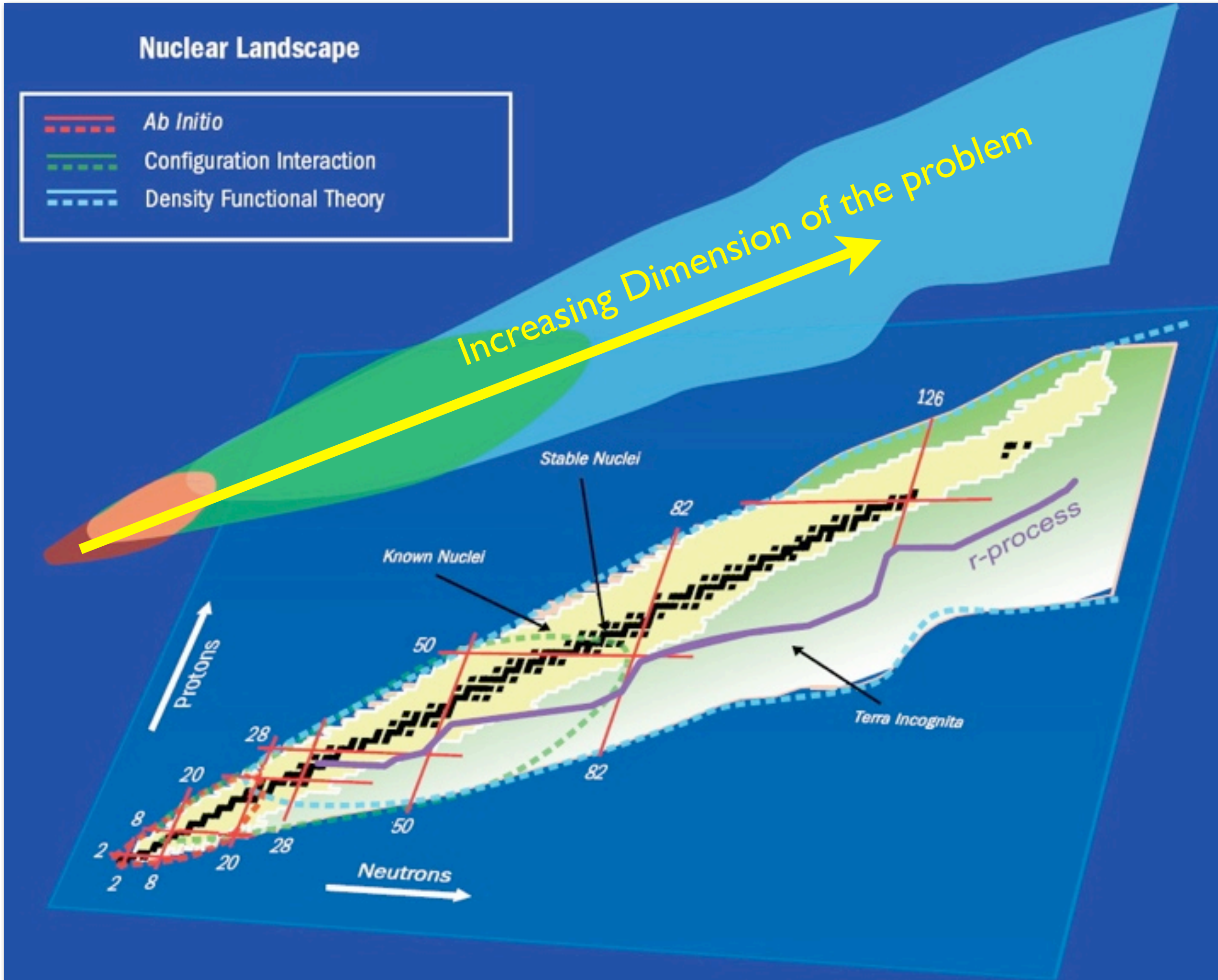
(Received 10 January 1973)

We examine the convergence rate of the sum over intermediate-particle states in the second-order core-polarization diagram of the effective shell-model interaction. For a G matrix resulting from the Reid soft-core interaction, convergence is achieved in an oscillator basis only after the intermediate particle is summed over five or six major-shell excitations ($10\hbar\Omega$ to $12\hbar\Omega$ excitations). The total effect of this diagram on the shell-model spectra of ^{18}O is markedly altered from the results of Kuo and Brown and others who only include oscillator excitations of one major shell ($2\hbar\Omega$) in the second-order diagram. We further demonstrate that slow convergence is attributed to strong components of the effective tensor force in the G matrix.

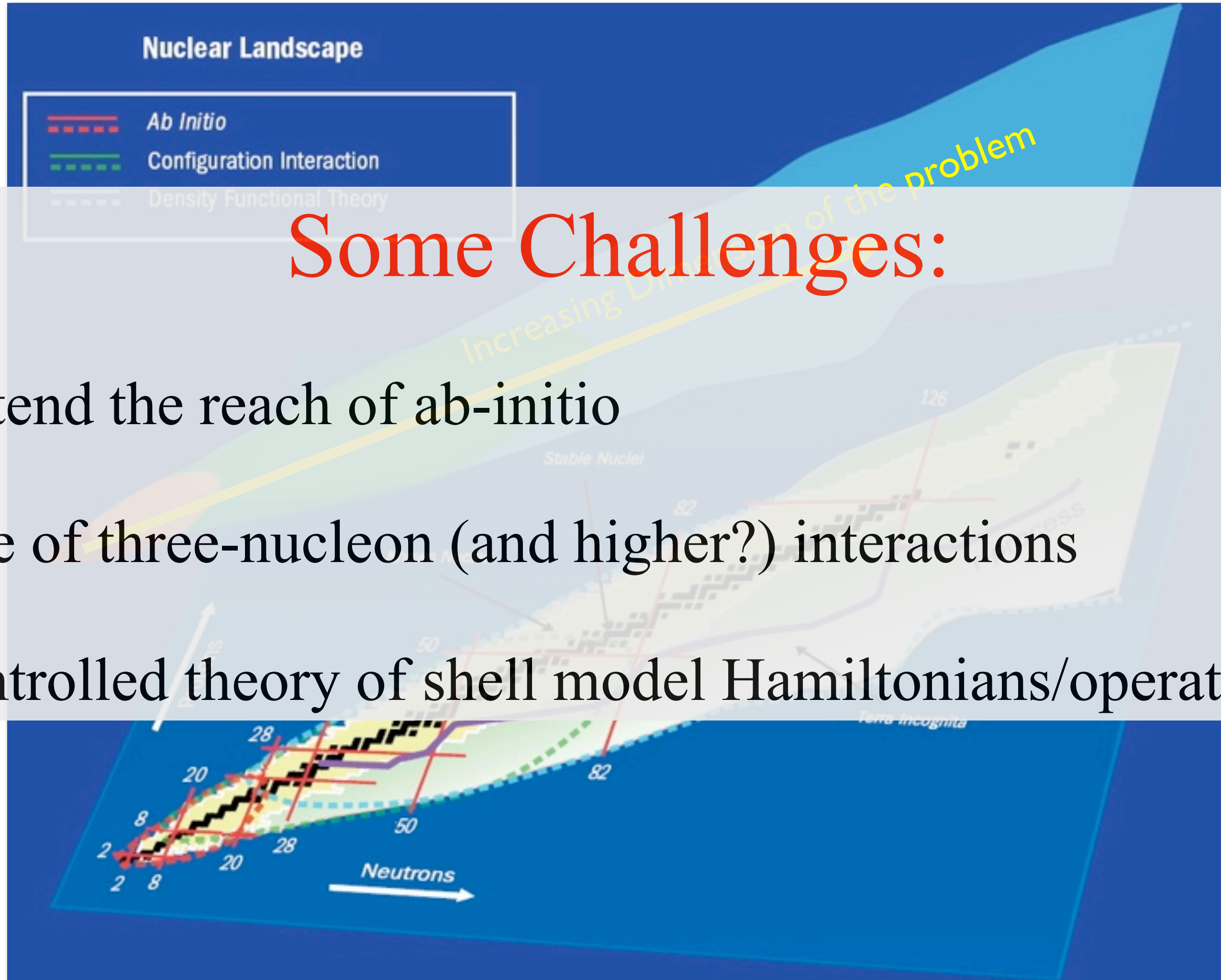
Happy Birthday James. You were right in spite of what Gerry said!

The nuclear many-body landscape



Calculate the properties of thousands of strongly-interacting nuclei rooted in the underlying QCD

The nuclear many-body landscape



Some Challenges:

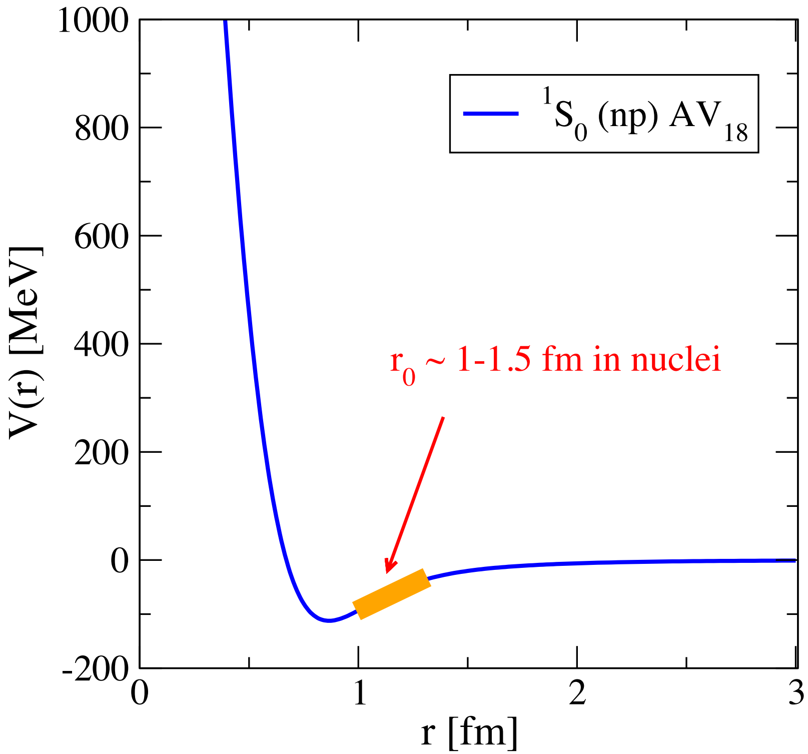
1) Extend the reach of ab-initio

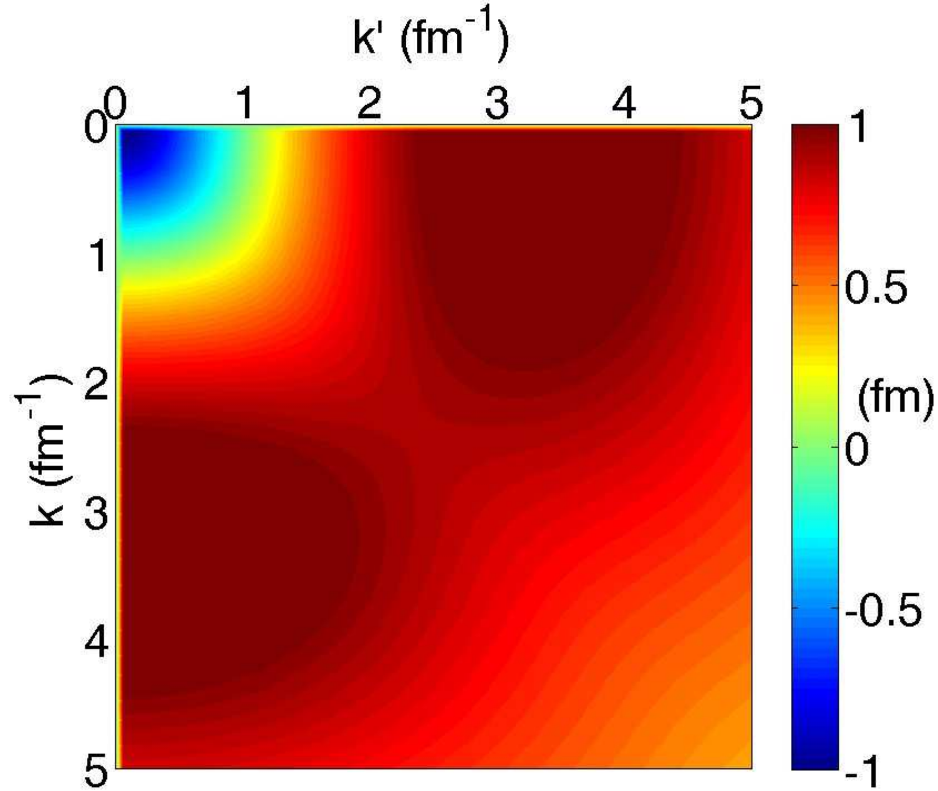
2) role of three-nucleon (and higher?) interactions

3) controlled theory of shell model Hamiltonians/operators

Calculate the properties of thousands of strongly-interacting nuclei rooted in the underlying QCD

Scale-dependent sources of non-perturbative physics

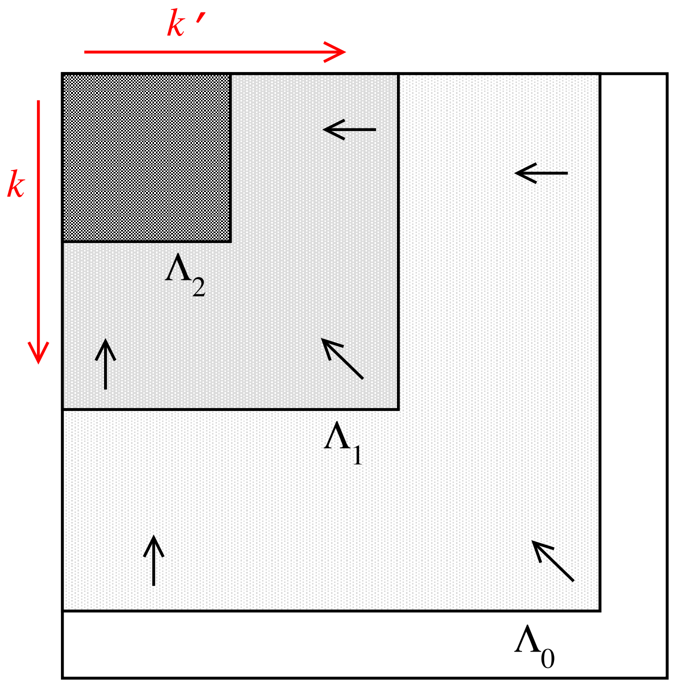




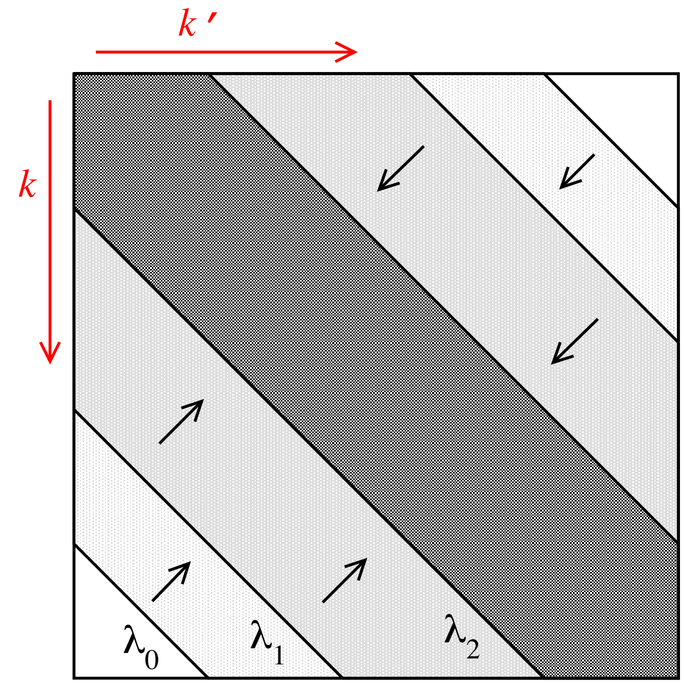
low and high k modes strongly coupled

Complications: strong correlations, non-perturbative, poorly convergent basis expansions, ...

2 Types of Renormalization Group Transformations



“$V_{\text{low k}}$”



“Similarity RG”

Same consequences despite differences in appearance (Decoupling)

The Similarity Renormalization Group

Wegner, Glazek and Wilson

Unitary transformation via flow equations:

$$\frac{dH_\lambda}{d\lambda} = [\eta(\lambda), H_\lambda] \qquad \text{with} \qquad \eta(\lambda) \equiv \frac{dU(\lambda)}{d\lambda} U^\dagger(\lambda)$$

Engineer η to do different things as λ => 0

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

$$\eta(\lambda) = [\mathcal{G}_\lambda, H_\lambda]$$

$$\mathcal{G}_\lambda = T \;\Rightarrow\; H_\lambda \text{ driven towards diagonal in k} - \text{space}$$

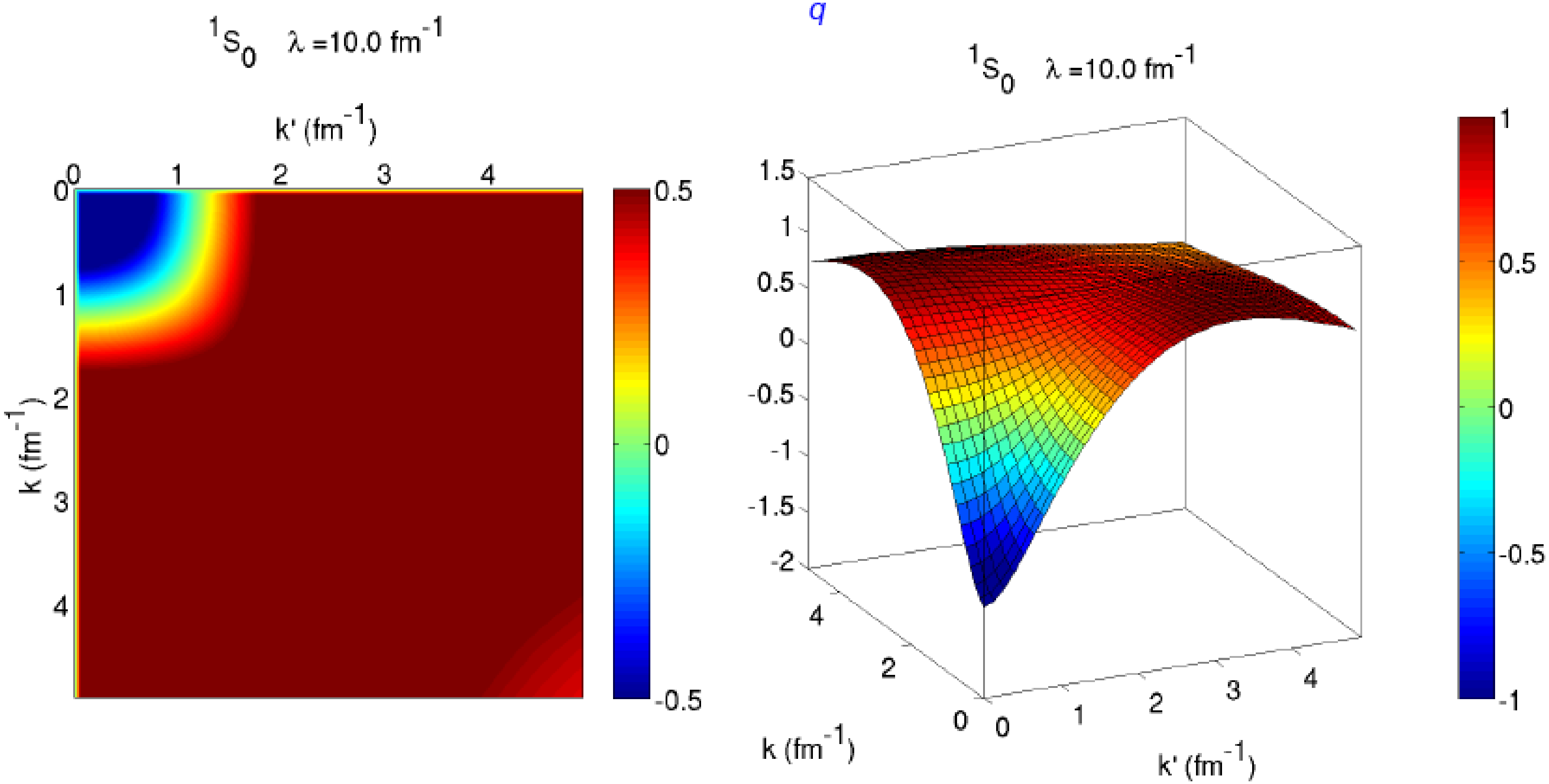
$$\mathcal{G}_\lambda = PH_\lambda P + QH_\lambda Q \;\Rightarrow\; H_\lambda \text{ driven to block} - \text{diagonal}$$

$$\vdots$$

SRG evolved NN interactions with η = [T,H]

- In each partial wave with $\epsilon_k = \hbar^2 k^2/M$ and $\lambda^2 = 1/\sqrt{s}$

$$\frac{dV_\lambda}{d\lambda}(k,k') \propto -(\epsilon_k - \epsilon_{k'})^2 V_\lambda(k,k') + \sum_q (\epsilon_k + \epsilon_{k'} - 2\epsilon_q) V_\lambda(k,q) V_\lambda(q,k')$$

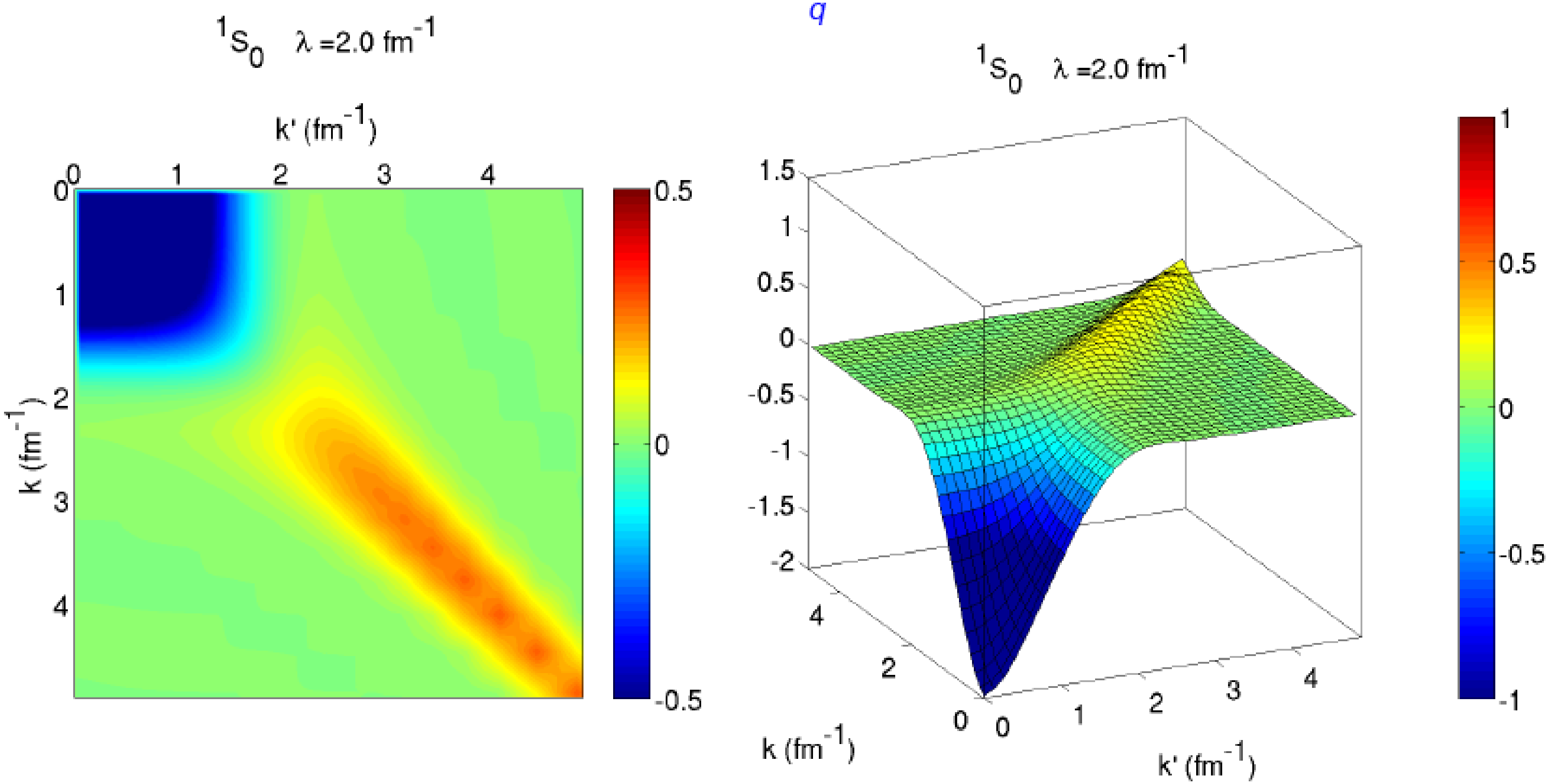


λ = 10.0 fm^{-1}

SRG evolved NN interactions with $\eta = [T,H]$

- In each partial wave with $\epsilon_k = \hbar^2 k^2/M$ and $\lambda^2 = 1/\sqrt{s}$

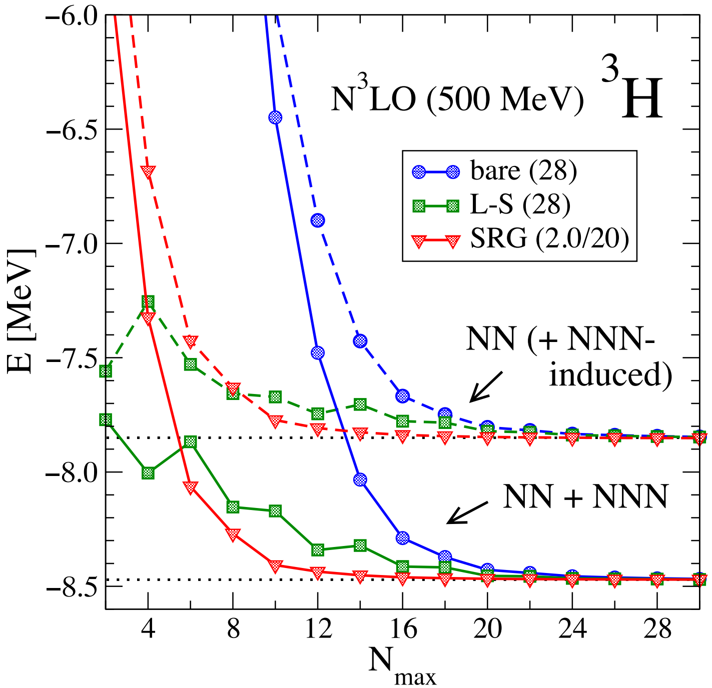
$$\frac{dV_\lambda}{d\lambda}(k,k') \propto -(\epsilon_k - \epsilon_{k'})^2 V_\lambda(k,k') + \sum_q (\epsilon_k + \epsilon_{k'} - 2\epsilon_q) V_\lambda(k,q) V_\lambda(q,k')$$

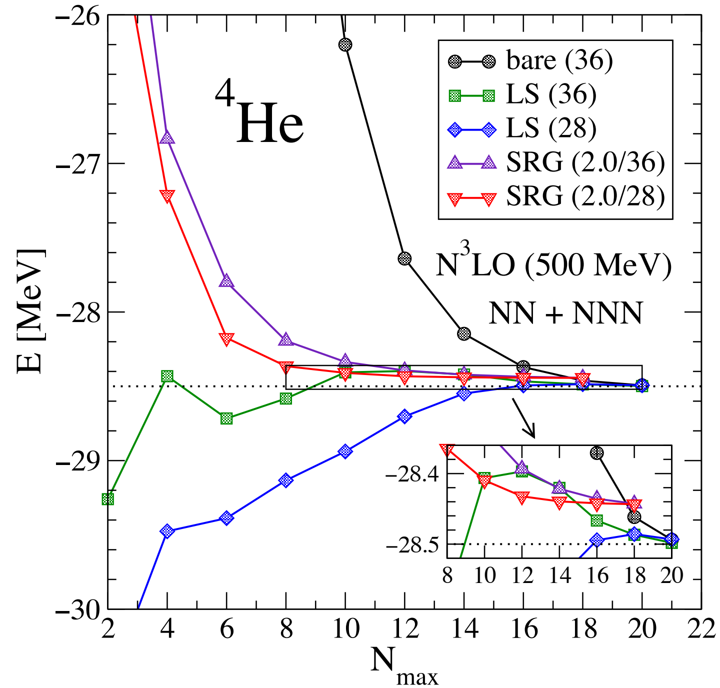


λ = 2.0 fm^{-1}

Simplifications at low resolutions

Jurgenson, Furnstahl, Navratil PRL 103 (2009)





- decoupling drastically improves convergence
- SRG evolution induces many-body forces: inclusion of three-body sector has been achieved
  (Jurgenson, Furnstahl, Navratil, PRL 103, 082501; Hebeler, PRC 85, 021002)

Free space versus in-medium evolution

Free space SRG: $V(\lambda)_{2N}$ fixed in 2N system
$V(\lambda)_{3N}$ fixed in 3N system

$\vdots$

$V(\lambda)_{aN}$ fixed in aN system

Use $T + V(\lambda)_{2N} + V(\lambda)_{3N} + \ldots + V(\lambda)_{aN}$ in A-body system

In-medium SRG:
evolution done at finite density (i.e., directly in A-body system).

Different mass regions => different SRG evolutions

inconvenience outweighed (?) by simplifications allowed by normal-ordering

Normal Ordered Hamiltonians

Pick a reference state Φ (e.g., HF) and apply Wick's theorem to 2nd-quantized Hamiltonian

$$
\begin{aligned}
A_i A_j A_k A_l \cdots A_m &= N(A_i A_j A_k A_l \cdots A_m) \\
&+ N\Big((\overbrace{A_i A_j} A_k A_l \cdots A_m) + \text{all other single contractions} \Big) \\
&+ N\Big((\overbrace{A_i A_j}\,\overbrace{A_k A_l} \cdots A_m) + \text{all other double contractions} \Big) \\
&\vdots \\
&+ N\Big((\text{all fully contracted terms} \Big)
\end{aligned}
$$

$$\overbrace{a_i^\dagger a_j} = \delta_{ij}\theta(\epsilon_F - \epsilon_i) \qquad \overbrace{a_i a_j^\dagger} = \delta_{ij}\theta(\epsilon_i - \epsilon_F)$$

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

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) :

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

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

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

0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N (See R. Roth's talk)

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

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0-, 1-, 2-body terms contain some 3NF effects thru density dependence => Efficient truncation scheme for evolution of 3N? (See R. Roth's talk)

In-medium SRG for Nuclear matter

- Normal order H w.r.t. non-int. fermi sea
- Choose SRG generator to eliminate "off-diagonal" pieces

$$\frac{dH(s)}{ds} = [\eta(s), H(s)]$$

$$\eta = [\hat{f}, \hat{\Gamma}]$$

$$\lim_{s \to \infty} \Gamma_{od}(s) = 0$$

$$\langle 12|\Gamma_{od}|34\rangle = 0 \text{ if } \mathrm{f}_{12} = \mathrm{f}_{34}$$

- Truncate to 2-body normal-ordered operators "IM-SRG(2)"

$$H(\infty) = E_{vac}(\infty) + \sum f_i(\infty) N(a_i^\dagger a_i) + \frac{1}{4}\sum [\Gamma_d(\infty)]_{ijkl} N(a_i^\dagger a_j^\dagger a_l a_k)$$

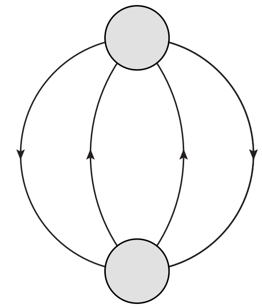
$$\begin{aligned} E_{vac}(\infty) &\rightarrow E_{gs} \\ f_k(\infty) &\rightarrow \epsilon_k \text{ (fully dressed s.p.e.)} \\ \Gamma_d(\infty) &\rightarrow f(k', k) \text{ (Landau q.p. interaction)} \end{aligned}$$

Microscopic realization of SM ideas: dominant MF + weak A-dependent NN_{eff}

In-medium SRG Equations Infinite Matter

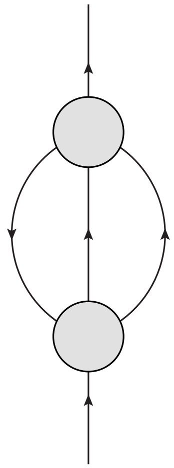
0-body flow

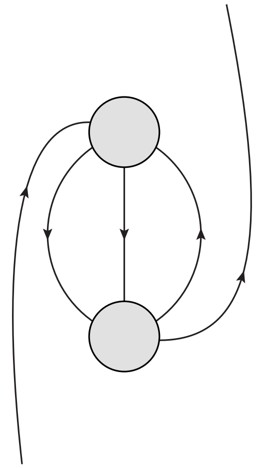
$$\frac{d}{ds}E_{vac} = \frac{1}{2}\sum_{ijkl}(f_{ij} - f_{kl})|\langle ij|\Gamma|kl\rangle|^2\, n_i n_j \bar{n}_k \bar{n}_l$$



1-body flow

$$\frac{d}{ds}f_a = \sum_{bcd}(f_{ad} - f_{bc})|\langle ad|\Gamma|bc\rangle|^2\left(\bar{n}_b\bar{n}_c n_d + n_b n_c \bar{n}_d\right)$$



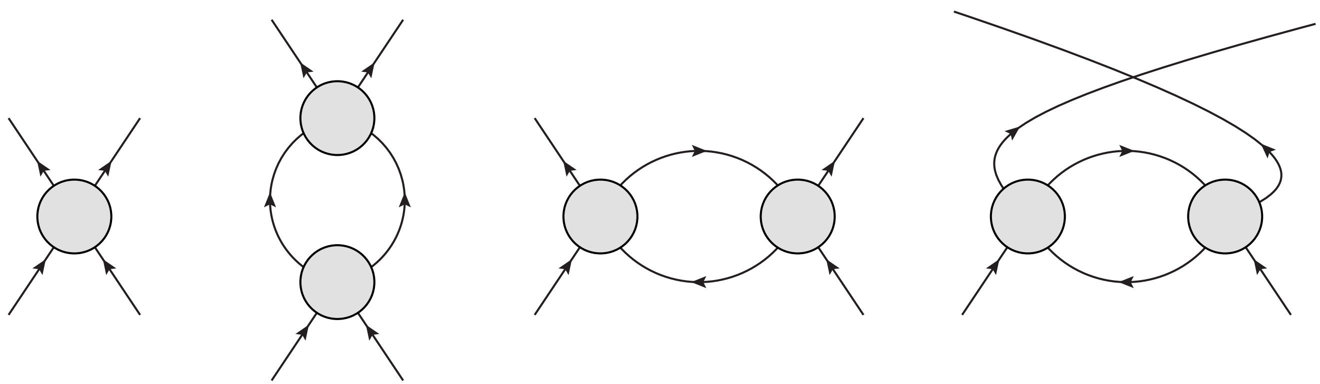


interference of 2p1h 2h1p self-energy terms

In-medium SRG Equations Infinite Matter

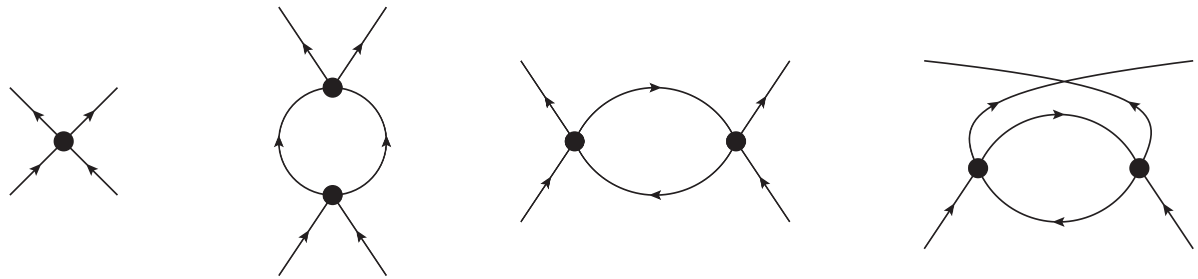
2-body flow

$$
\begin{aligned}
\langle 12|\frac{d\Gamma}{ds}|34\rangle &= -(f_{12}-f_{34})^2\langle 12|\Gamma|34\rangle \\
&+ \frac{1}{2}\sum_{ab}(f_{12}+f_{34}-2f_{ab})\,\langle 12|\Gamma|ab\rangle\langle ab|\Gamma|34\rangle\big(1-n_a-n_b\big) \\
&+ \sum_{ab}\big[(f_{1a}-f_{3b})-(f_{2b}-f_{4a})\big]\langle 1a|\Gamma|3b\rangle\langle b2|\Gamma|a4\rangle(n_a-n_b) \\
&- \sum_{ab}\big[(f_{2a}-f_{3b})-(f_{1b}-f_{4a})\big]\langle 2a|\Gamma|3b\rangle\langle b1|\Gamma|a4\rangle(n_a-n_b)
\end{aligned}
$$



Note the interference between s, t, u channels a-la Parquet theory

SRG is manifestly non-perturbative

$\Gamma(\delta s) \sim$ 

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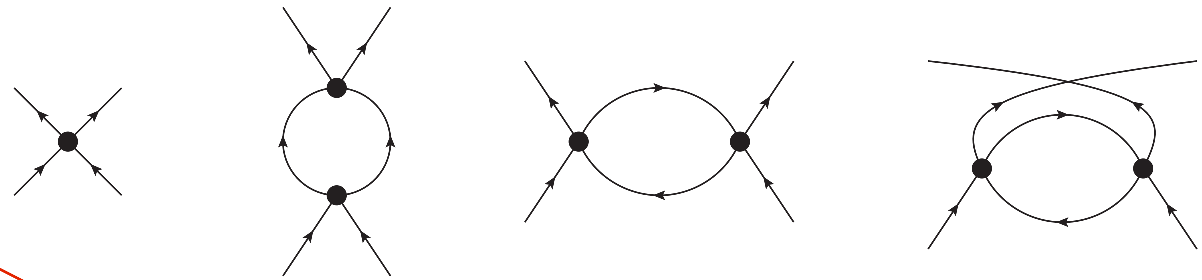
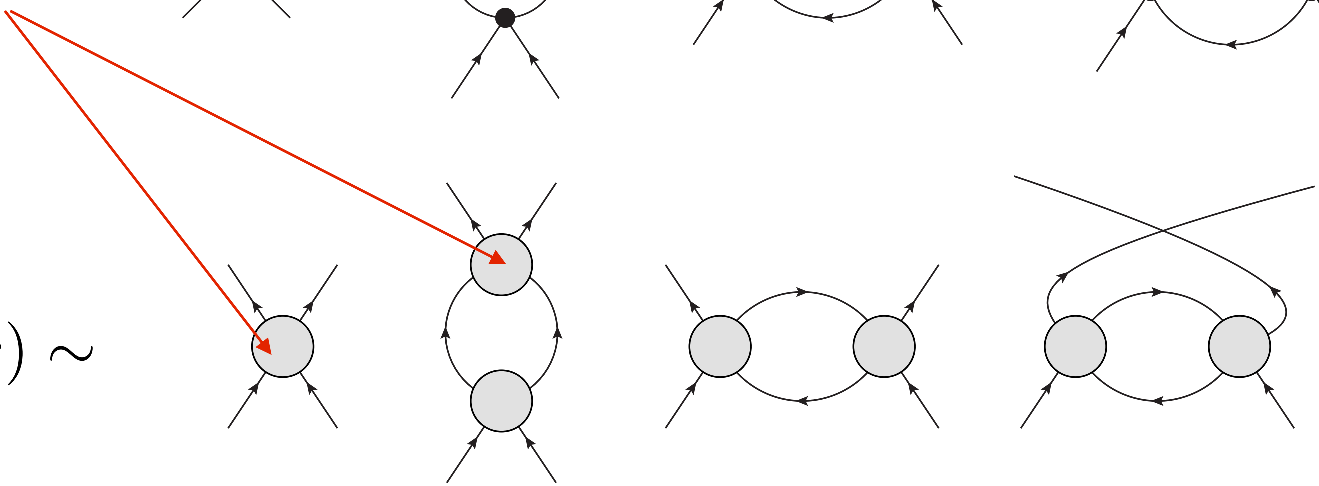


$$\Gamma(2\delta s) \sim$$



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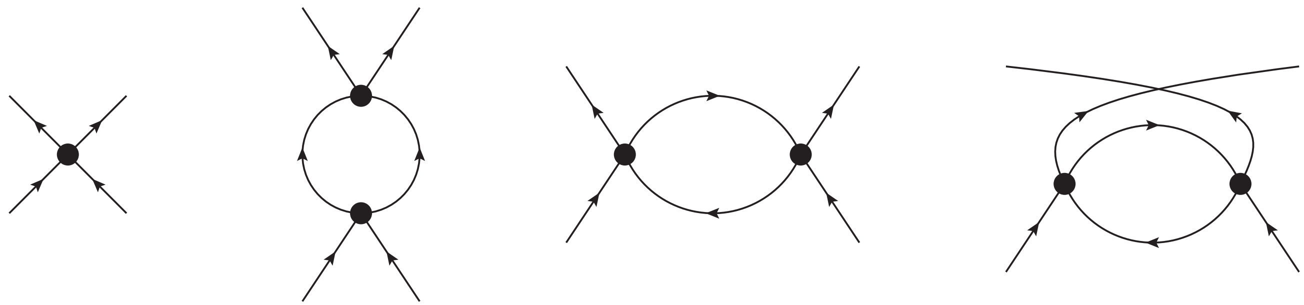
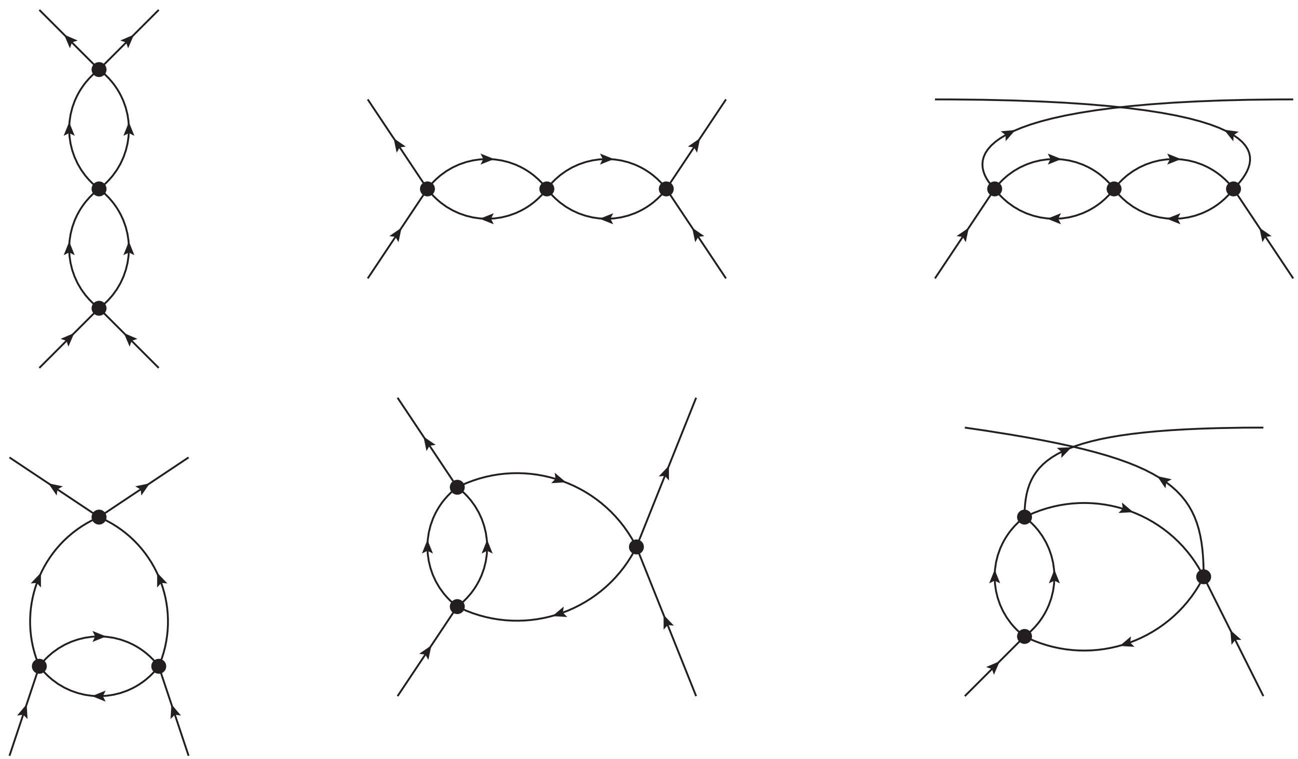
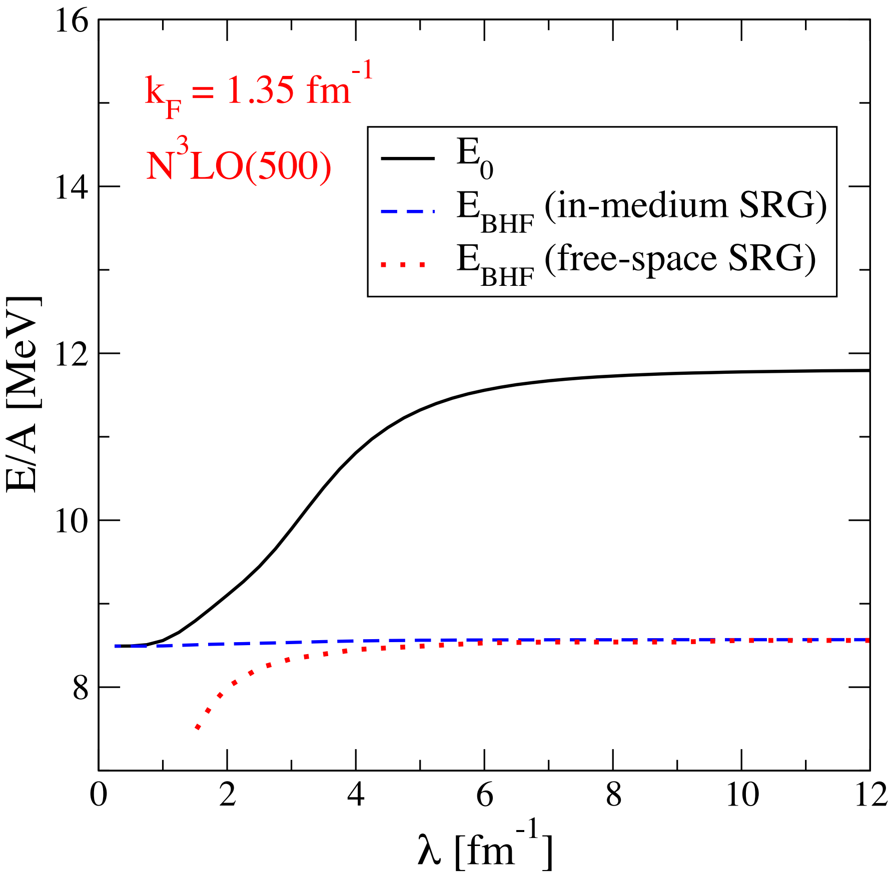


$\Gamma(2\delta s) \sim$

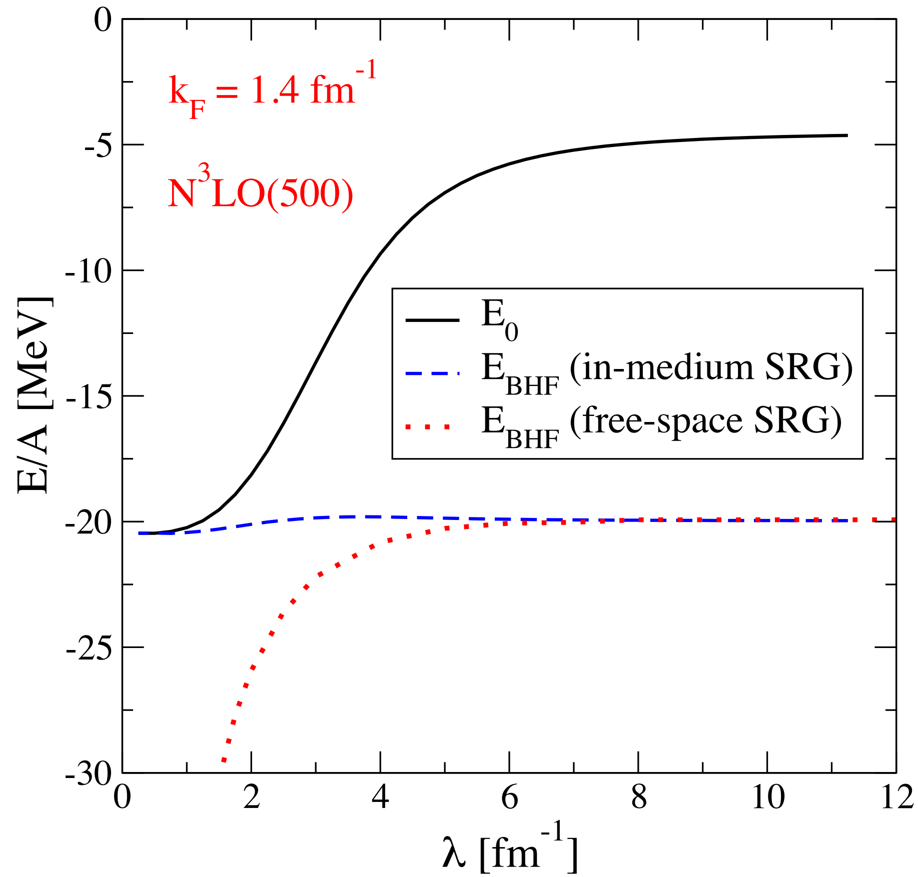


+ many more ...

Correlations "adiabatically" summed into H(λ)



PNM*

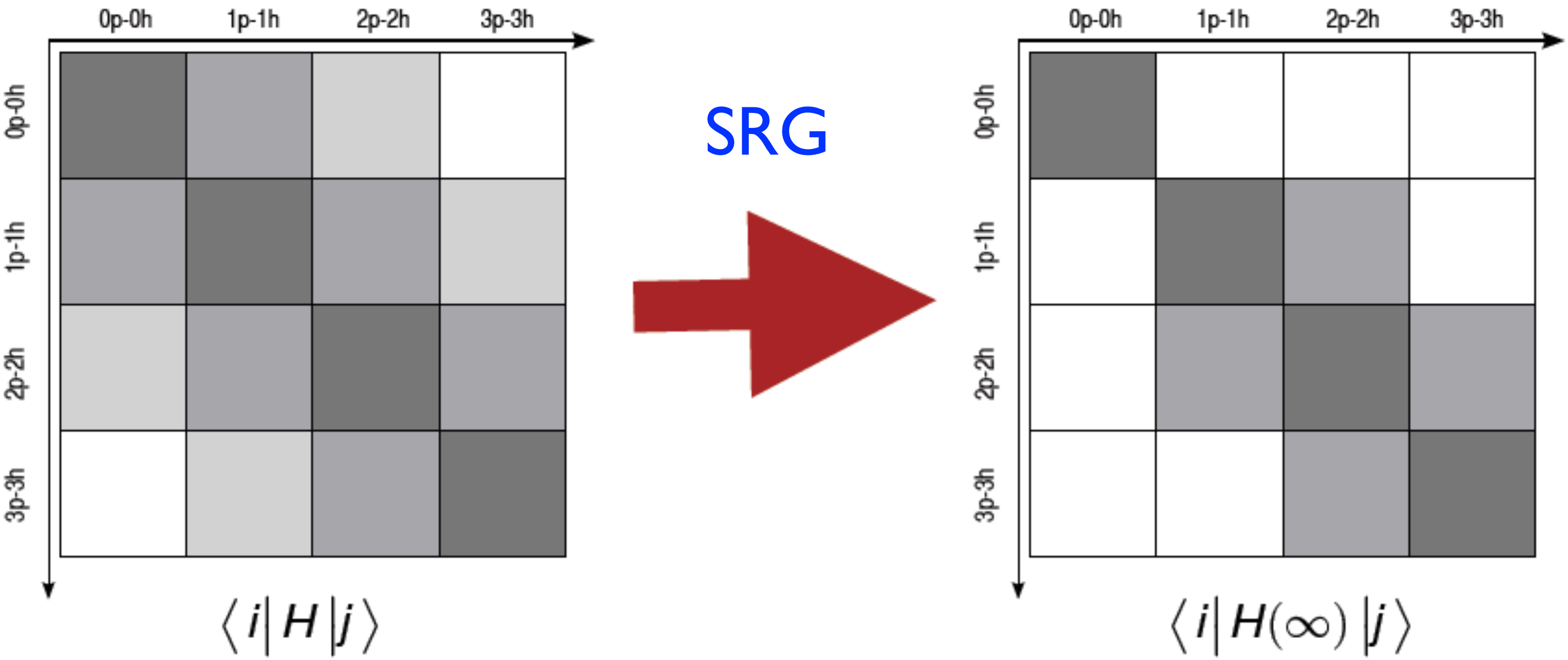


SNM*

Weak cutoff dependence over large range => dominant 3,4,...-body terms evolved implicitly

*Neglects ph-channel.

In-medium SRG for closed-shell nuclei (g.s.)



aim: decouple reference state (0p-0h) from excitations

$\Gamma_{od} = \Gamma_{pp'hh'} + \text{h.c}$

$f_{od} = f_{ph} + \text{h.c.}$

Choice of Generator

- Wegner

$$\eta^{I} = [H^{d}, H^{od}]$$

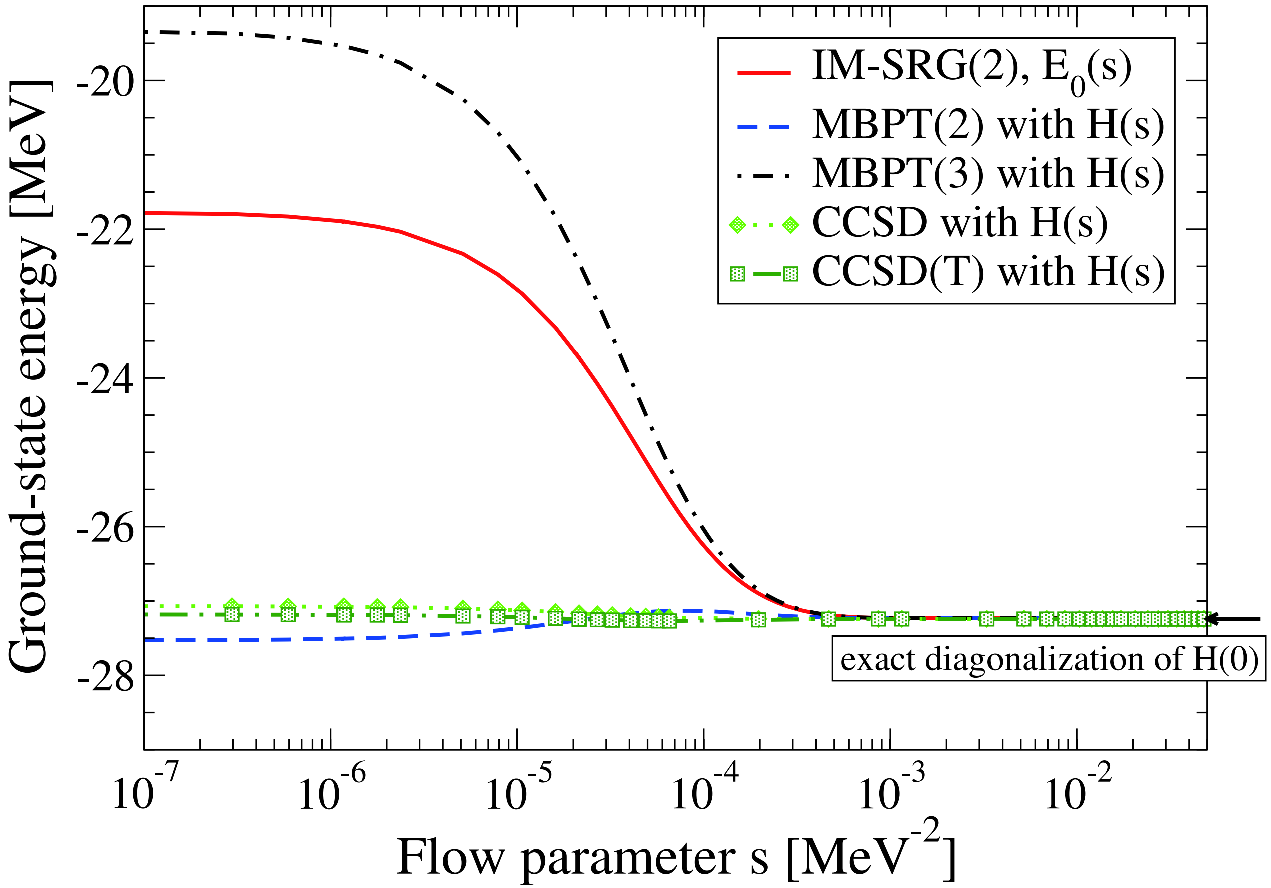
- White (J. Chem. Phys. 117, 7472)

$$\eta^{II} = \sum_{ph} \frac{f_h^p}{E_p - E_h} :A_h^p: + \sum_{pp'hh'} \frac{\Gamma_{hh'}^{pp'}}{E_{pp'} - E_{hh'}} :A_{hh'}^{pp'}: + \text{H.c.}$$

$E_p - E_h, E_{pp'} - E_{hh'}$: approx. 1p1h, 2p2h excitation energies

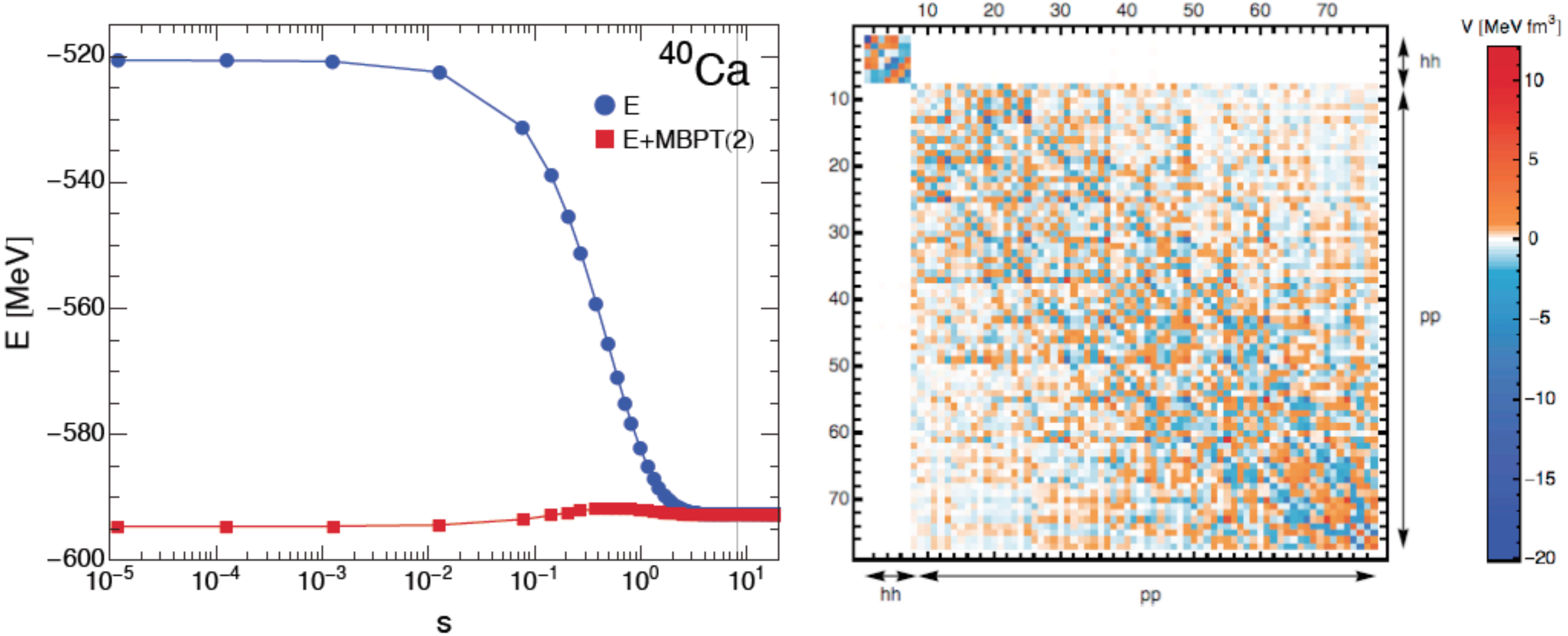
- off-diagonal matrix elements are suppressed like $e^{-\Delta E^2 s}$ (Wegner) or e^{-s} (White)
- g.s. energies ($s \to \infty$) for both generators agree within a few keV

Resummation of correlations into zeroth order E_0



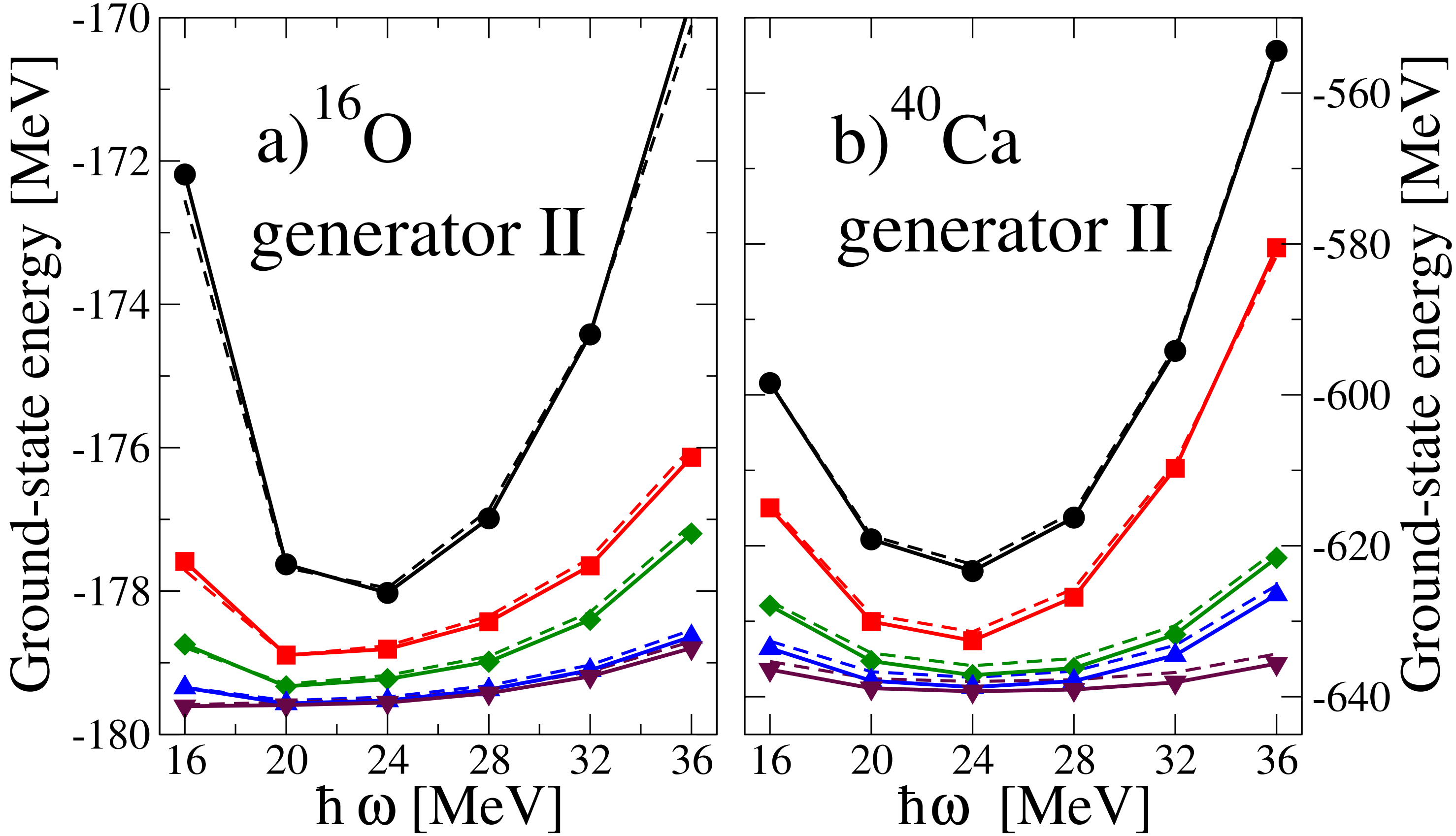
K. Tsukiyama, SKB, A. Schwenk, PRL 106 (2011).

Resummation of correlations into zeroth order E_0



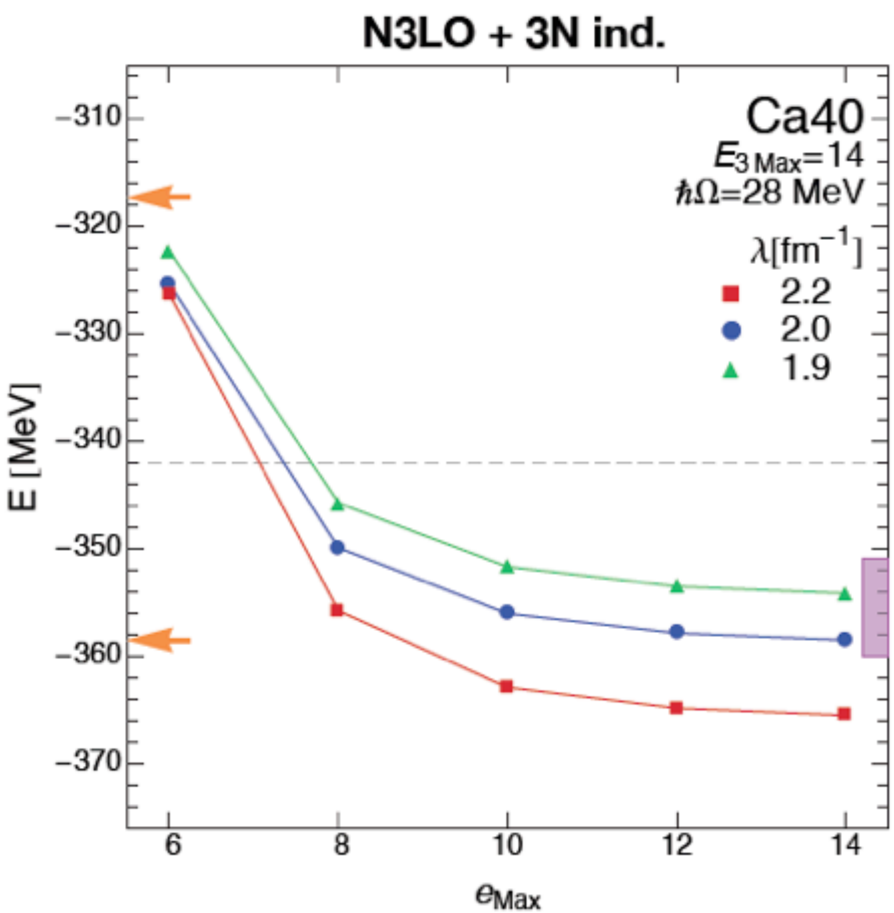
$V_{\text{SRG}}(\text{N3LO}), \lambda = 2.0\ \text{fm}^{-1}, e_{\text{Max}} = 8$

IM-SRG to diagonalize many-body problems



- good agreement with CCSD(T)
- N^6 scaling with number of s.p. orbitals

Using free-space SRG NN + NNN(induced) input

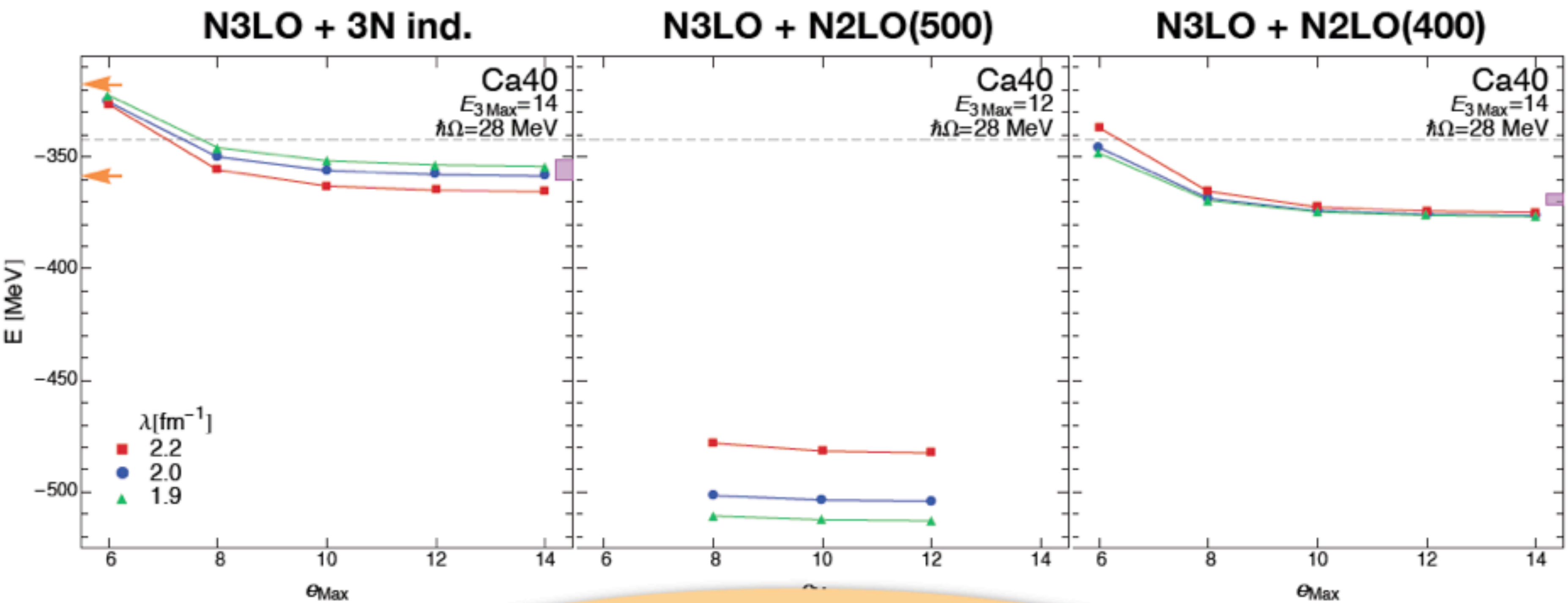


H. Hergert et al., PRC 87 (2013)

CCSD/Λ-CCSD(T), $\lambda = \infty$, G. Hagen et al., PRL 109, 032502 (2012)

CCSD, $\lambda = 1.9 - 2.2$ fm^{-1} , S.Binder, R.Roth et al., in preparation & PRL 109, 052501 (2012)

H. Hergert et al., PRC 87 (2013)



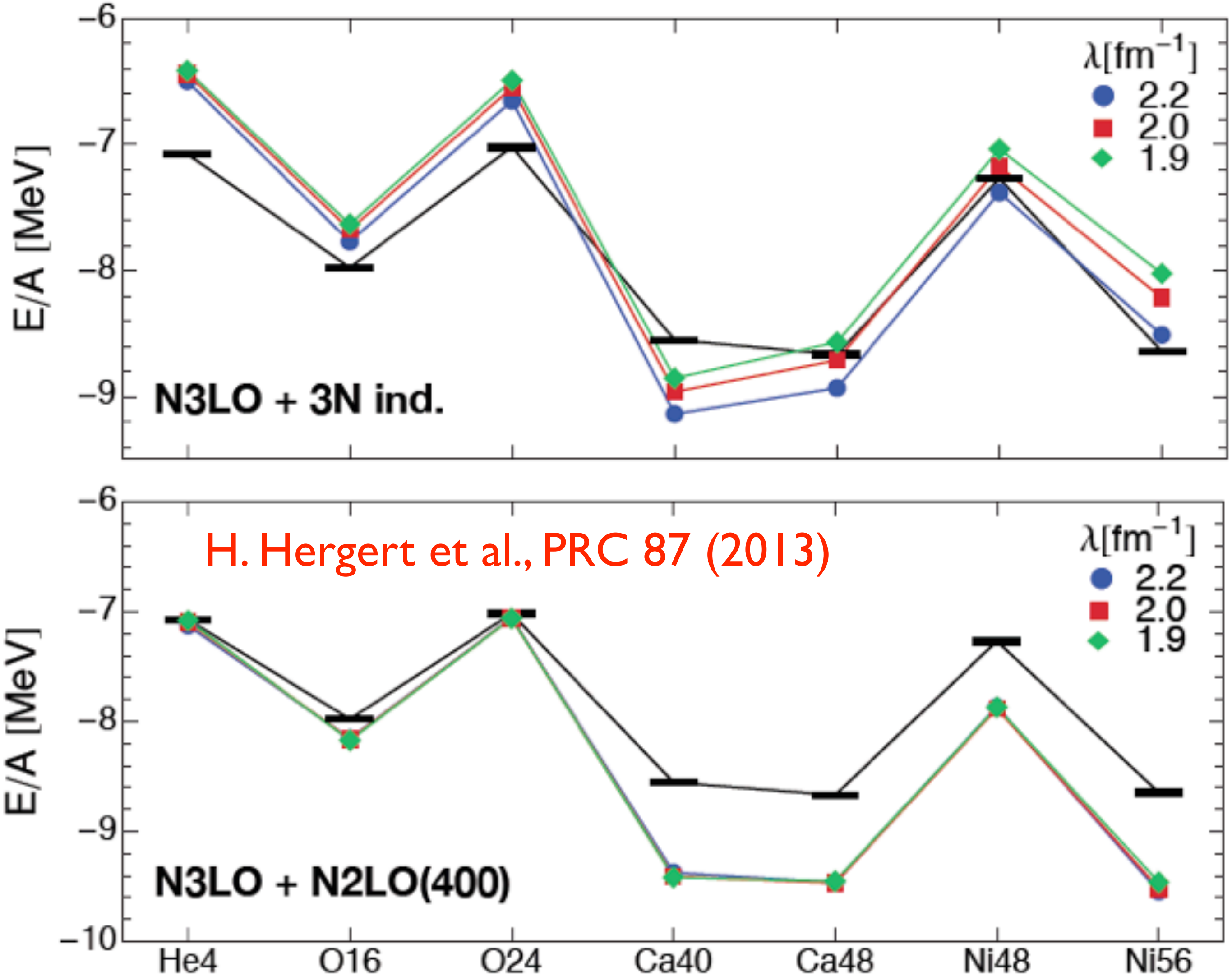
constraints & diagnostics for chiral Hamiltonians

(cf. talk by R. Roth)

CCSD/Λ-CCSD(T), $\lambda = \infty$, G. Hagen et al., PRL 109, 032502 (2012)

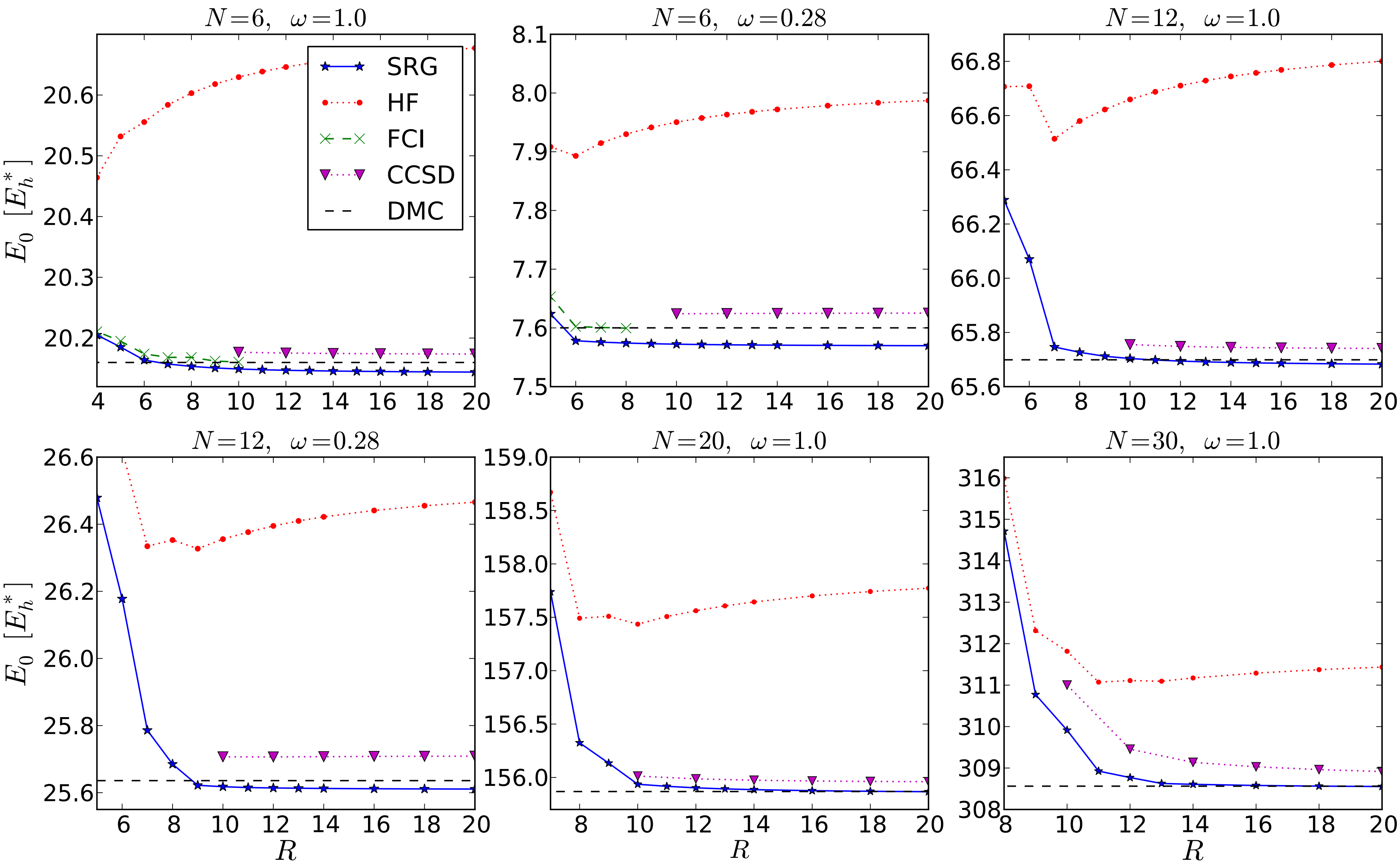
CCSD, $\lambda = 1.9 - 2.2$ fm^{-1} , S.Binder, R.Roth et al., in preparation & PRL 109, 052501 (2012)

Importance of initial NNN forces



extrapolation method: R. Furnstahl, G. Hagen & T. Papenbrock, PRC 86,031301 (2012)

Application to Quantum Dots



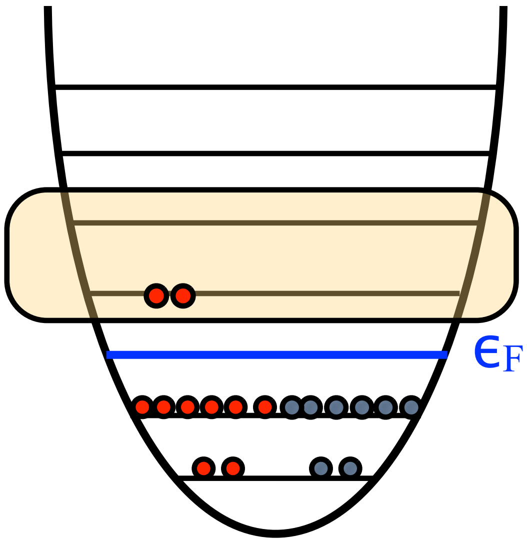
Curiosity: higher accuracy than CCSD (both n^6 methods)

IM-SRG for open-shell nuclei

- use IM-SRG to derive effective Hamiltonians & operators for Shell Model calculations
  (K. Tsukiyama, S.K. Bogner, A. Schwenk, PRC 85, 061304 (2012))

- use IM-SRG directly with suitable open-shell reference state: H. Hergert et al., arXiv:1302.7294
  - multi-reference state from m-scheme Hartree-Fock, (small-scale) Shell Model, DMRG, etc.
  - Hartree-Fock-Bogoliubov many-body state

In-medium SRG for open shell nuclei (Shell model)



inactive particle orbitals q_i

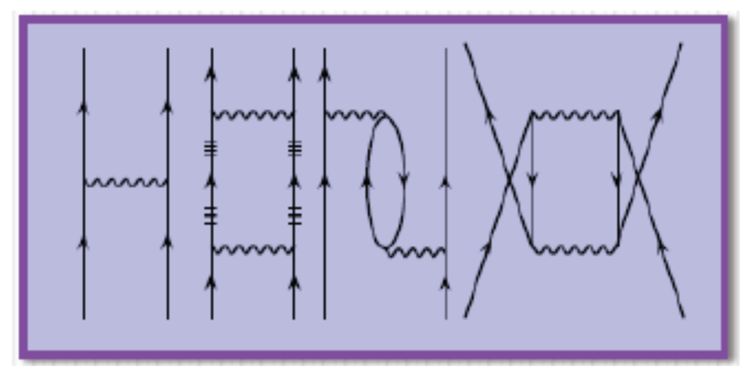
active valence orbitals v_i

inactive hole orbitals h_i

Decouple valence orbitals and diagonalize:

$$PH_{eff}P|\Psi\rangle = (E - E_c)P|\psi\rangle$$

Previously, H_{eff} from MBPT and empirical corrections



Can we use the IM-SRG to do this?

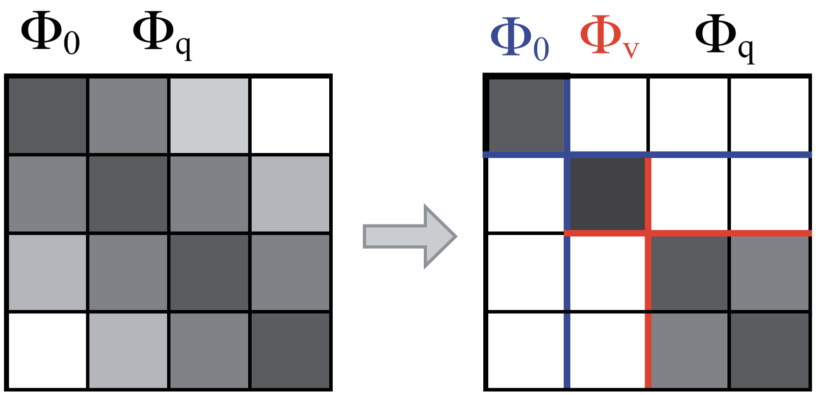
In-medium SRG recipe for shell model

1) Identify all terms in H that don't annihilate model-space states

$$\hat{O}_i \left(\mathrm{v}_1^\dagger \ldots v_{N_v}^\dagger |\phi\rangle \right) \neq 0$$

2) Solve flow equations

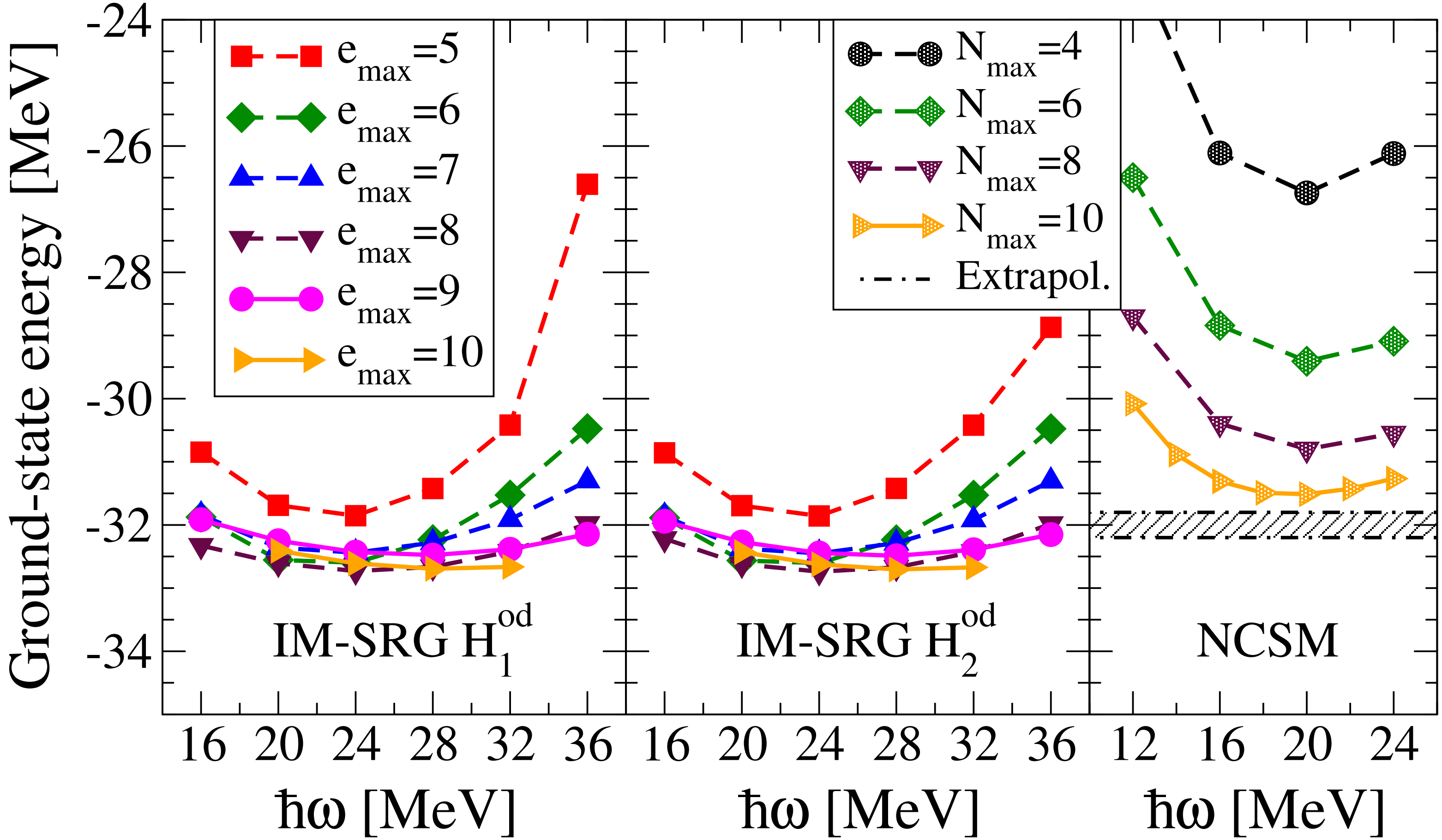
$$\frac{dH}{ds} = [\eta, H]$$
$$\eta = [H^{(od)}, H]$$
$$H^{(od)} = \sum g_i \hat{O}_i$$



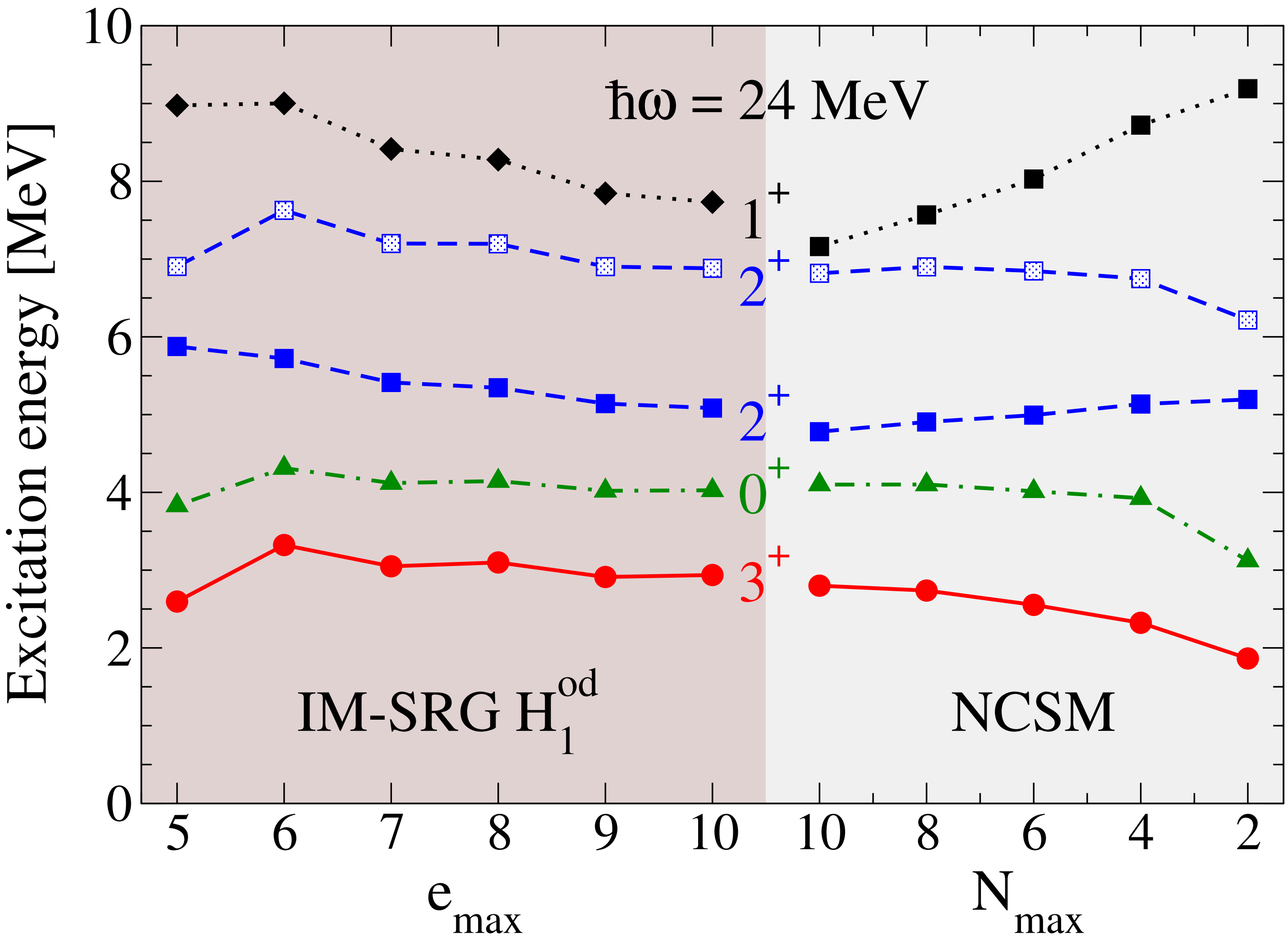
3) Diagonalize fully-evolved H in the reduced valence space

$$PH(\infty)P|\Psi\rangle = (E - E_c)P|\psi\rangle$$

^{6}Li ground state: comparison to exact NCSM



^{6}Li spectra: comparison to NCSM



Summary

- RG methods can simplify many-body calculations immensely **provided that induced many-body operators are under control**

- In-medium evolution + truncations based on normal-ordering => simple way to evolve dominant induced 3, 4, ...A-body interactions with 2-body machinery

- Can be used as ab-initio method in and of itself, or to construct soft interactions for other ab-initio methods

- Extensions to shell model H_{eff}/O_{eff} look promising.

Example: Perturbative content of SRG

- Solve SRG eqn's to 2nd-order the bare coupling

$$E_0(s) \approx E_0(0) + \frac{1}{4} \sum_{1234} n_1 n_2 \bar{n}_3 \bar{n}_4 \frac{|V_{1234}(0)|^2}{f_{12} - f_{34}} \left(1 - e^{-s(f_{12}-f_{34})^2}\right)$$

$$E_{corr}(s) \approx \frac{1}{4} \sum_{1234} n_1 n_2 \bar{n}_3 \bar{n}_4 \frac{|V_{1234}(0)|^2}{f_{12} - f_{34}} e^{-s(f_{12}-f_{34})^2}$$

As s increases, contributions shuffled from correlation energy into
The non-interacting VEV contribution (I.e., Hartree-Fock)

Microscopic connection to shell model?
(MF + "weak" A-dependent residual NN interaction)