In-medium Similarity Renormalization Group for nuclear many-body systems

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HPCI project “Large-scale quantum many-body calculations for nuclear property and it’s application”

In collaboration with
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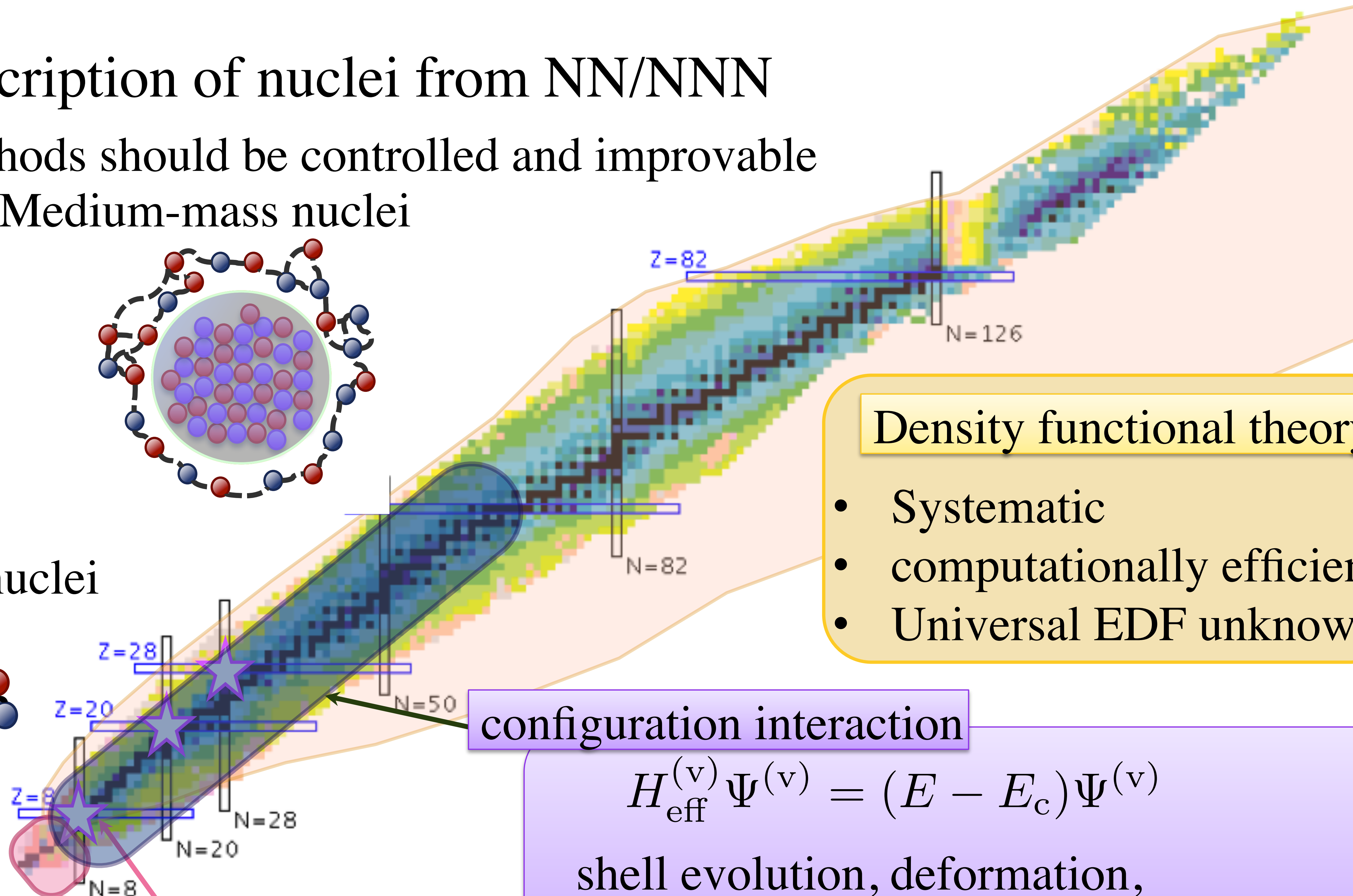
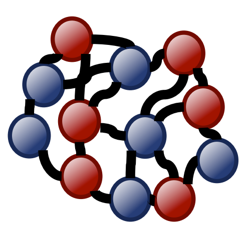
Description of nuclei from NN/NNN

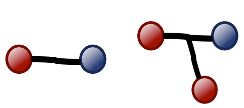
Methods should be controlled and improvable

Medium-mass nuclei



Light nuclei





NN/NNN

Density functional theory

- Systematic
- computationally efficient
- Universal EDF unknown

configuration interaction

$$H^{(\mathrm{v})}_{\mathrm{eff}}\Psi^{(\mathrm{v})} = (E - E_{\mathrm{c}})\Psi^{(\mathrm{v})}$$

shell evolution, deformation, double-bata decay,..

ab initio $H\Psi = E\Psi$

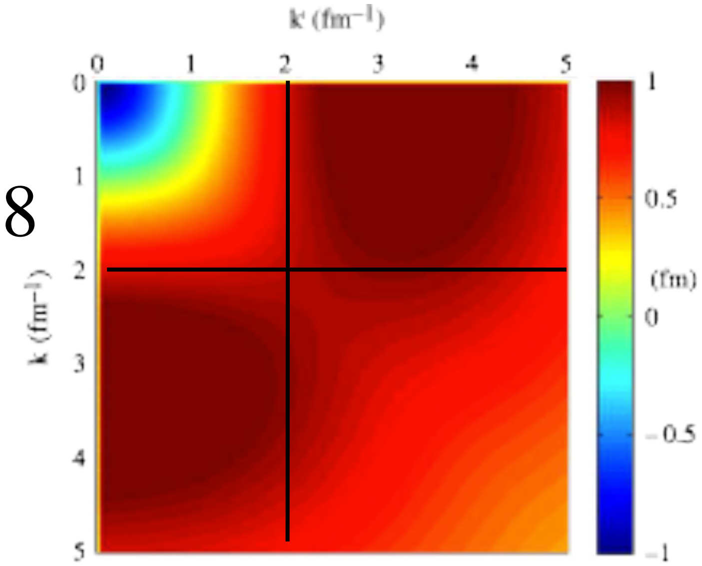
binding energy, radius

accuracy, feasibility

Λ QCD

V(k,k')

AV18

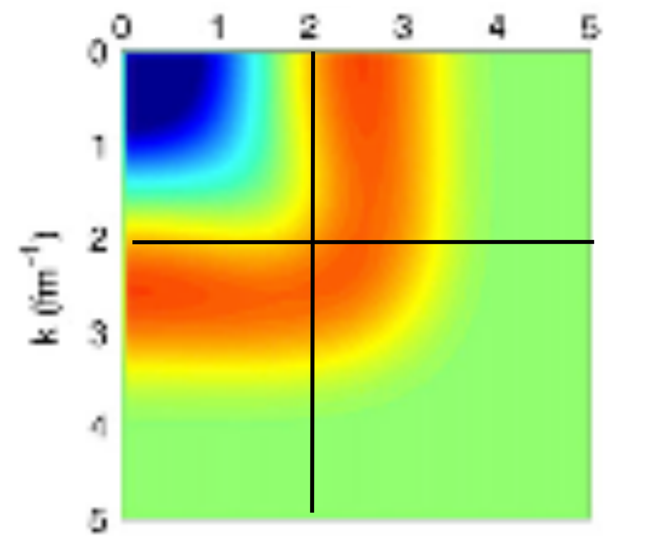


hard

$$H(\Lambda) = T_{\rm rel} + V_{2N}(\Lambda) + V_{3N}(\Lambda) + V_{4N}(\Lambda) + \cdots$$

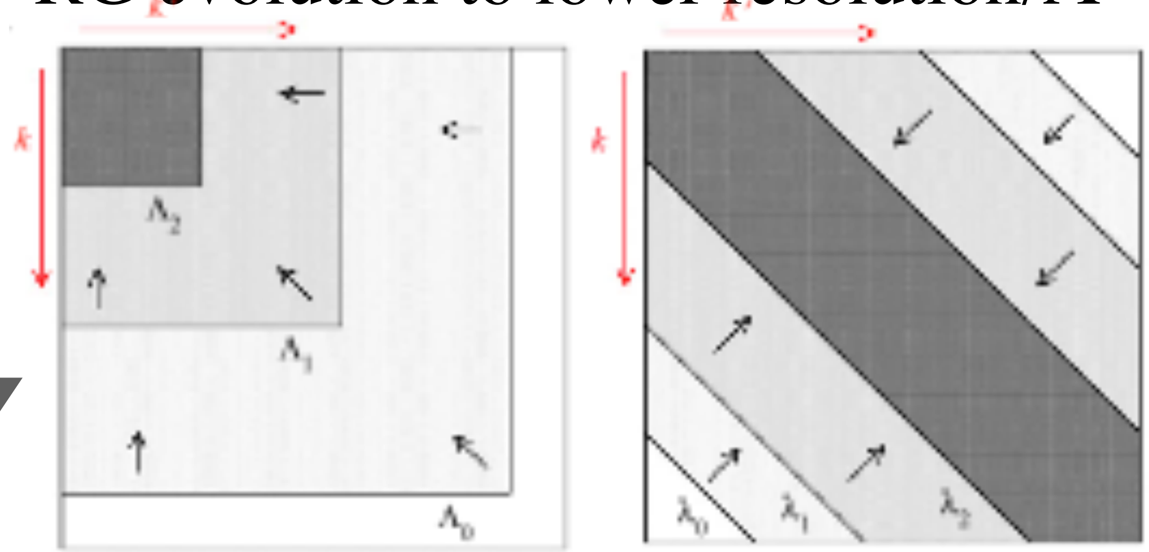
χEFT

pion-exchange and short-range contact
power counting (still open)
-systematic expansion
-many-body forces automatically



still hard

RG evolution to lower resolution/Λ



NN observables kept unchanged

Low-momentum interactions
$V_{\text{low-k}}$, SRG

Bogner-Schwenk-Furnstahl, PPNP, 65, 94 (2010)

Similarity Renormalization Group

Glazek and Wilson, Phys. Rev. D**48**, 5863(1993), or Wegner, Ann. Phys. (Leipzig) **3**, 77 (1994)

The unitary evolution of the Hamiltonian via flow equation

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

$$\eta(s) = \frac{dU(s)}{ds}U^\dagger(s)$$

$$\Rightarrow \quad H(s) = U(s)HU^\dagger(s) \equiv \underline{H^d(s) + H^{od}(s)}$$

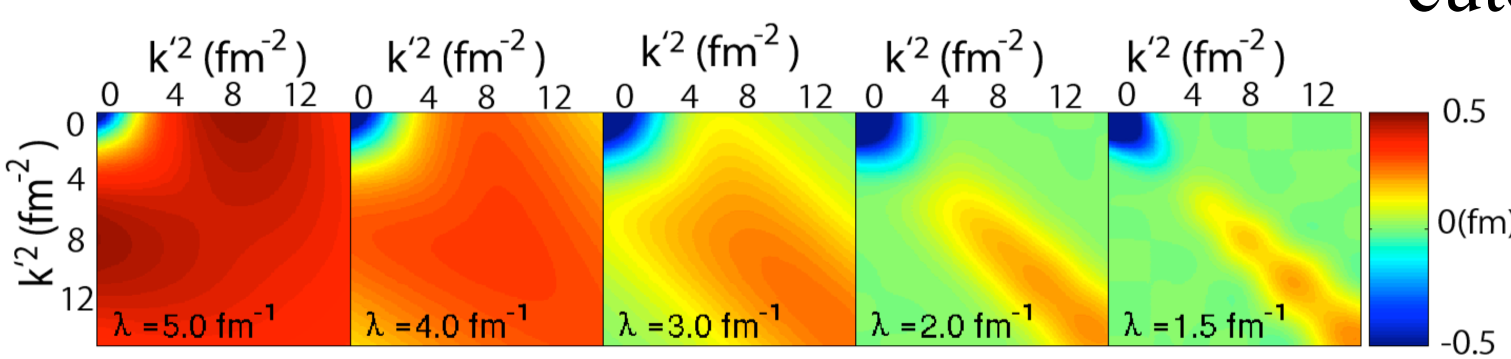
can arbitrarily be defined

$$\eta(s) = [H(s), H^{\mathrm{od}}(s)]$$ by F. Wegner $$\Rightarrow \quad \frac{d}{ds}\mathrm{Tr}\left\{\left(H^{\mathrm{od}}\right)^2\right\} \leq 0$$

Flexibility of choosing the $H^d(s)$ for a particular problem.

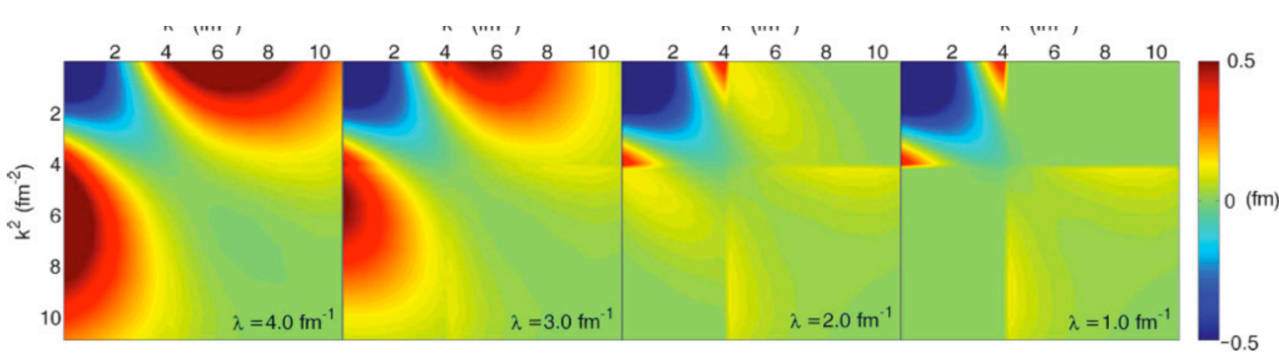
$\longrightarrow$ lower λ

cutoff $\lambda \equiv s^{-1/4}$ as evolution variable



$$H^d(s) = T$$

Bogner et al, PRC75, 061001(R) (2007)

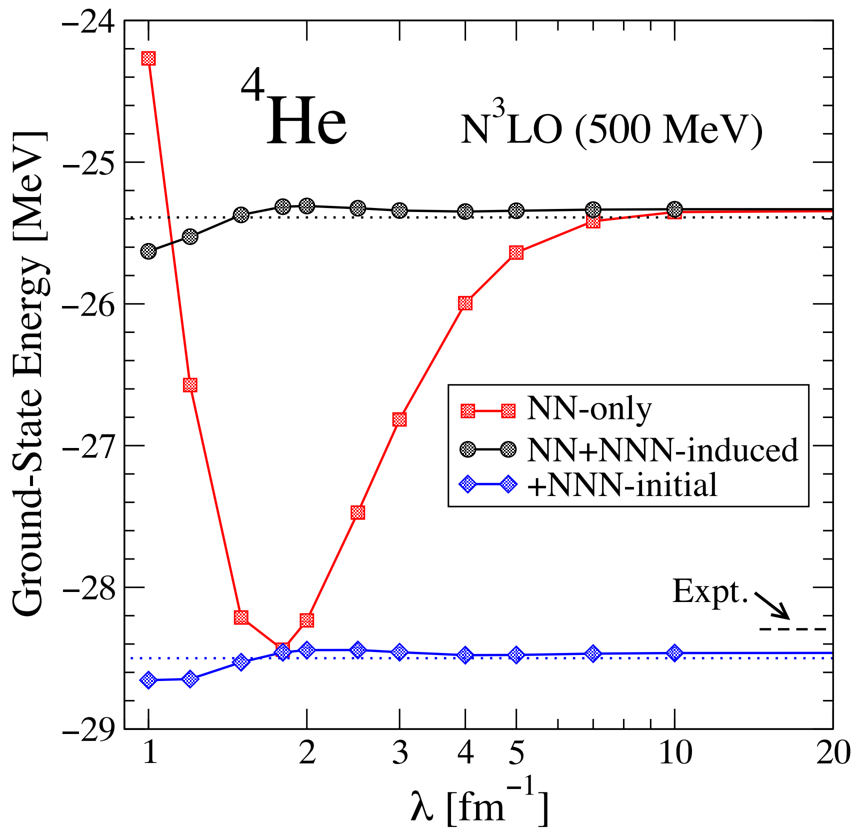


$$H^d(s) = \begin{pmatrix} PH(s)P & 0 \\ 0 & QH(s)Q \end{pmatrix}$$

Anderson et al, PRC77, 037001 (2008)

RG and many-body interactions

Free-space SRG, evolving consistent 3N interactions => exact method



- NN only => λ-dependent
- + induced NNN => almost λ-independent

Jurgenson, Furnstahl and Navratil PRL103, 082501(2009)

same trend for heavier systems

Roth et al., PRL107, 07201(2011)

$$H(s) = U(s)H^{(2)}U^{\dagger}(s) = \tilde{H}^{(2)}(s) + \underline{\tilde{H}^{(3)}(s) +} \cdots$$

<u>In-medium SRG</u>

- Defined in many-body system (finite density)
- Approximate evolution of 3-, .. A-body operators within 2b machinery.
- Different SRG evolutions for different mass regions.

K.T., S. Bogner and A. Schwenk, PRL106, 222502(2011)

Normal-ordered Hamiltonian

$$\hat{H} = \sum_{ij} T_{ij} a_i^\dagger a_j + \frac{1}{2!^2} \sum_{ijkl} V^{(2)}_{ijkl} a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{3!^2} \sum_{ijklmn} V^{(3)}_{ijklnm} a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l + \cdots$$

Normal order w.r.t. a finite-density Fermi vacuum $|\Phi\rangle$, e.g. HF.

$$H = E_0 + \sum_{ij} f_{ij} \{a_i^\dagger a_j\} + \frac{1}{2!^2} \sum_{ijkl} \Gamma_{ijkl} \{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{3!^2} \sum_{ijklmn} W_{ijklmn} \{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}$$

where coefficients of normal-ordered operators are given by $\langle\Phi| \{A_i A_j \cdots\} |\Phi\rangle = 0$

$$E_0 = \langle\Phi| H |\Phi\rangle = \sum_k T_{kk} n_k + \frac{1}{2} \sum_{ij} V^{(2)}_{ijij} n_i n_j + \frac{1}{6} \sum_{ijk} V^{(3)}_{ijkijk} n_i n_j n_k$$

$$f_{ij} = T_{ij} + \sum_k V^{(2)}_{ikjk} n_k + \frac{1}{2} \sum_{kl} V^{(3)}_{ikljkl} n_k n_l$$

$$\Gamma_{ijkl} = V^{(2)}_{ijkl} + \frac{1}{4} \sum_m V^{(3)}_{ijmklm} n_m \qquad n_i \equiv \theta(\epsilon_F - \epsilon_i)$$

$$W_{ijklmn} = V^{(3)}_{ijklmn}$$

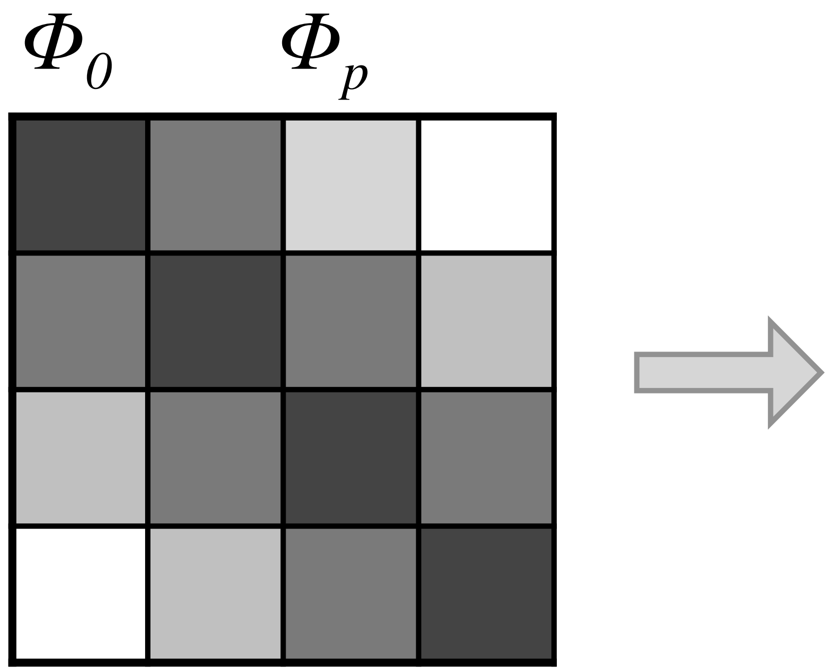
3-body and higher-body interactions through density- dependent coefficients.

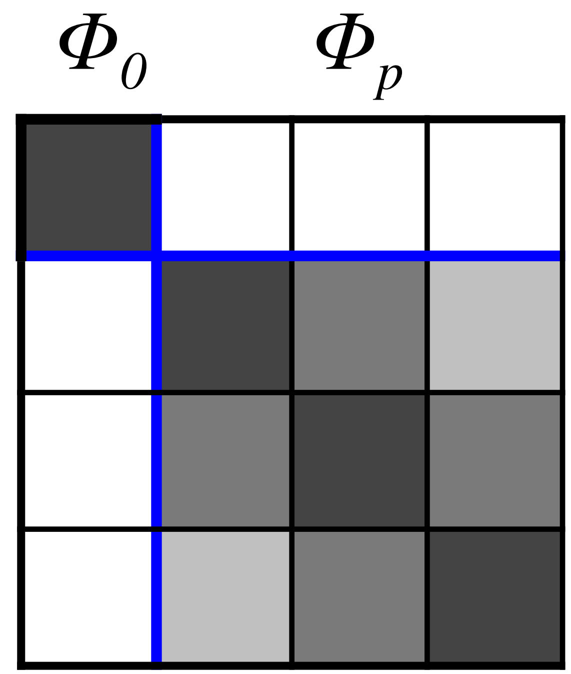
=> may be efficient truncation scheme

Decoupling (schematic picture)

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

η (s) is determined s as to eliminate $H^{\mathrm{od}}(s)$

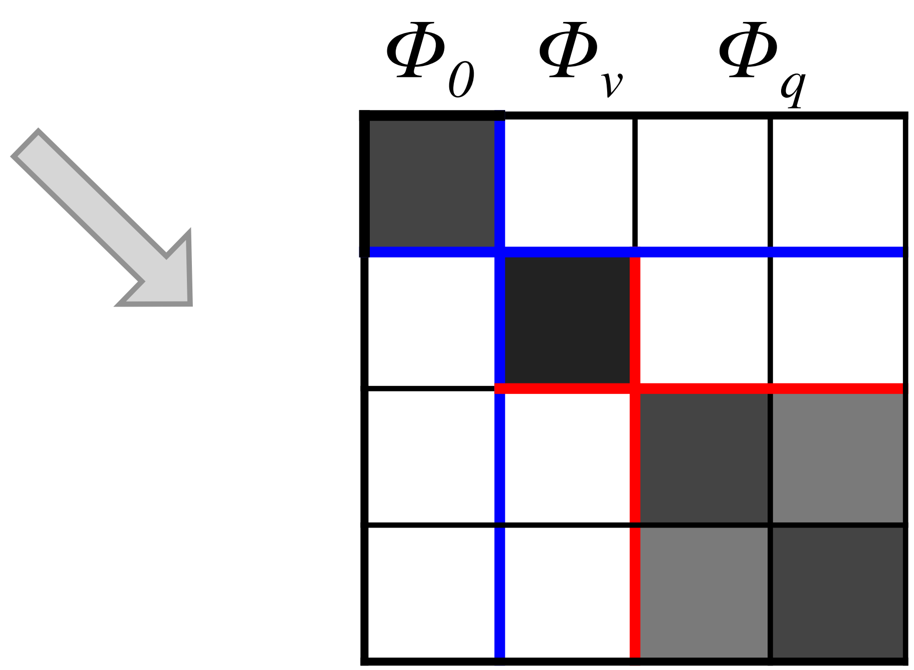




decouples ground state

$$H^{\mathrm{od}} = f_{\mathrm{ph}} + \Gamma_{\mathrm{pphh}}$$

vertices connecting reference state and *np-nh* excited states



decouples valence space

$$H^{od} = f_{ph} + \Gamma_{pphh} + f_{vq} + f_{vh} + \Gamma_{vv'qq'} + \Gamma_{vhpp'} + \Gamma_{vv'v''h}$$

vertices connecting valence space and outside of it.

In-medium SRG flow equation

$$\frac{dH(s)}{ds} = [\eta, H(s)] = [\eta^{(1)} + \eta^{(2)} + \eta^{(3)} + \cdots, f + \Gamma + W + \cdots]$$

commutator form => no unlinked diagram

=> <u>size extensive</u>: energy scales linearly w/ # of particles

IM-SRG(2): n^6, IM-SRG(3): n^8

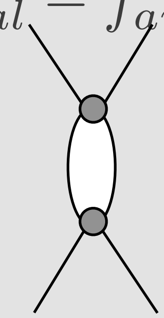
Flow eqns.

$$\boxed{\frac{d}{ds}E_0(s) = 2\sum_{ab} n_a \bar{n}_b \eta^{(1)}_{ab} f_{ba} + \frac{1}{2}\sum_{abcd} \eta^{(2)}_{abcd}\Gamma_{cdab}(s) n_a n_b \bar{n}_c \bar{n}_d}$$

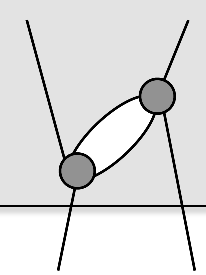
$$+ \frac{1}{18}\sum_{abcdef} \eta^{(3)}_{abcdef} W_{defabc} n_a n_b n_c \bar{n}_d \bar{n}_e \bar{n}_f$$

$$\frac{d}{ds}\Gamma_{ijkl}(s) = \sum_a \left\{(1-P_{ij})(\eta^{(1)}_{ia}\Gamma_{ajkl} - f_{ia}\eta^{(2)}_{ajkl}) - (1-P_{kl})(\eta^{(1)}_{ai}\Gamma_{ijal} - f_{ai}\eta^{(2)}_{ijal})\right\}$$

$$+ \frac{1}{2}\sum_{ab}\underline{(1-n_a-n_b)}(\eta^{(2)}_{ijab}\Gamma_{abkl} - \Gamma_{ijab}\eta^{(2)}_{abkl})$$ pp or hh



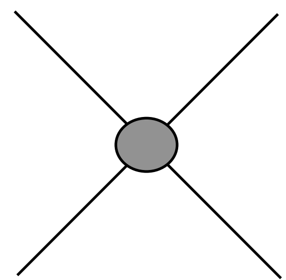
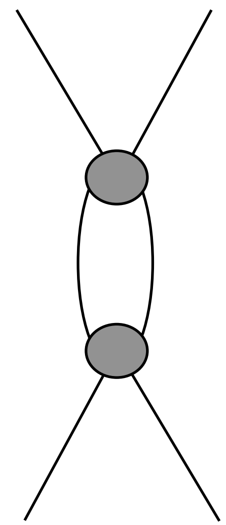
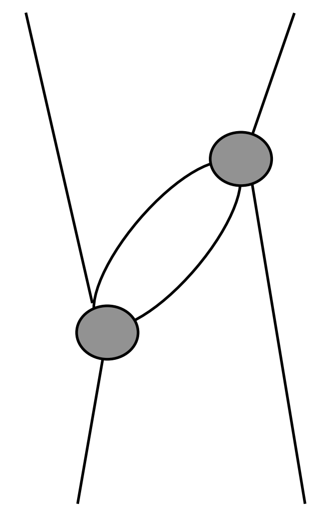
$$- \sum_{ab}\underline{(n_a - n_b)}\left[(1-P_{ij})(1-P_{kl})\eta^{(2)}_{bjal}\Gamma_{aibk}\right]$$ ph



$$+ \sum (n_a - n_b)\left(\eta^{(3)}_{aijbkl} f_{ba} - W_{aijbkl}\eta^{(1)}_{ba}\right)$$

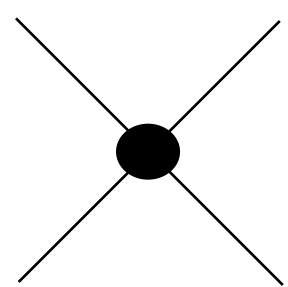
Non-Perturbative feature: Schematic

The flow equation can essentially be seen as

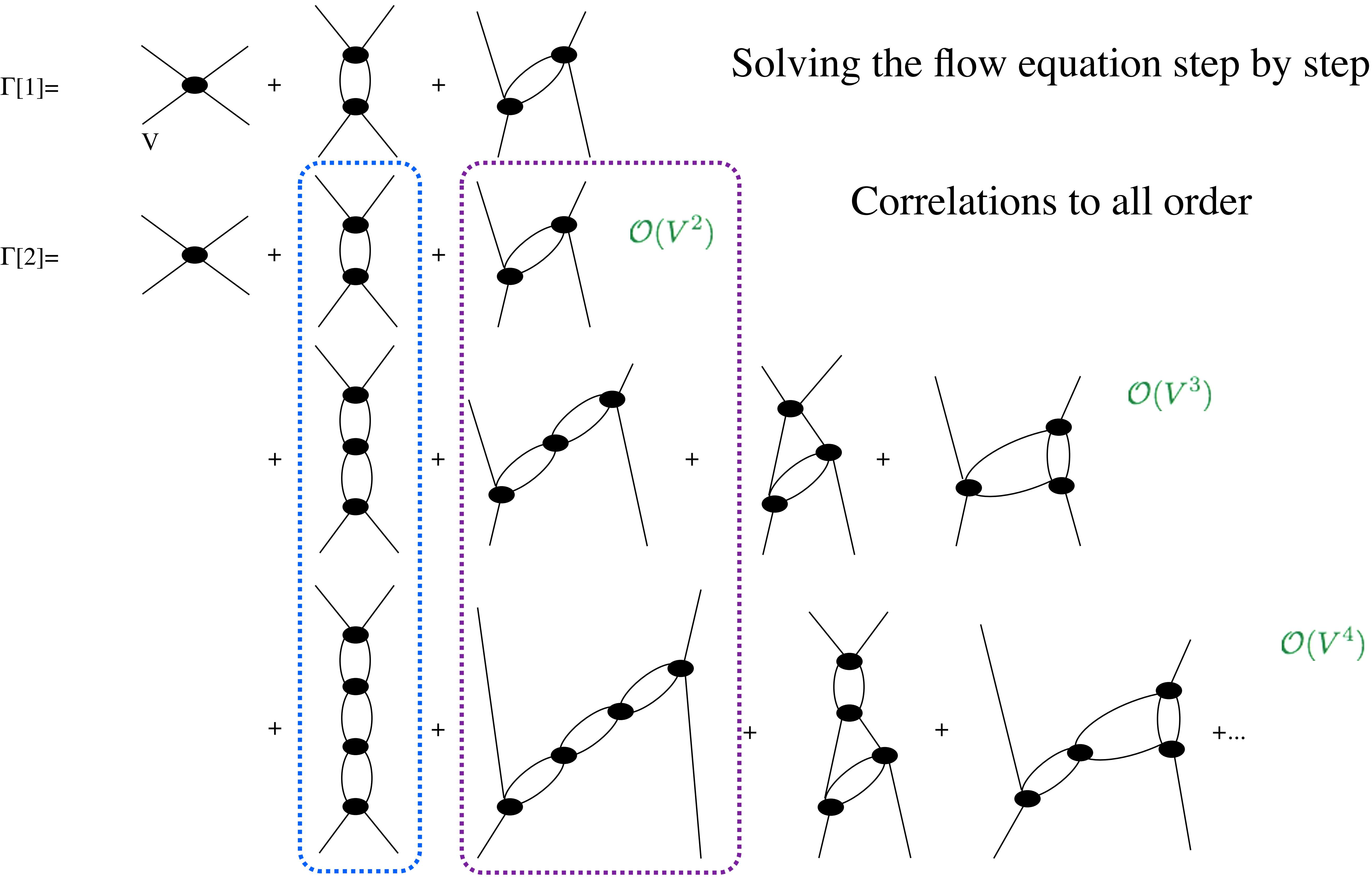
$\Gamma[n+1]=$  $+$  $+$ 

$\Gamma[n]$

With the initial condition

$\Gamma[0]=$  $=:$ V(bare two-body coupling)

Non-Perturbativeness of IM-SRG: Schematic



Solving the flow equation step by step

Correlations to all order

Flow equation by perturbative analysis

IM-SRG(2), 95%

IM-SRG(3), 99%

$$\dot{E}_0(s) = [\eta^{(2)},\Gamma]^{[2]} + [\eta^{(1)}, f]^{[4]} + [\eta^{(3)}, W]^{[4]}$$

$$\dot{f}(s) = [\eta^{(1)}, f]^{[2]} + [\eta^{(2)},\Gamma]^{[2]} + [\eta^{(1)},\Gamma]^{[3]} + [\eta^{(2)}, f]^{[3]} + [\eta^{(2)}, W]^{[3]} + [\eta^{(3)},\Gamma]^{[3]} + [\eta^{(3)}, W]^{[4]}$$

$$\dot{\Gamma}(s) = [\eta^{(2)}, f]^{[1]} + [\eta^{(2)},\Gamma]^{[2]} + [\eta^{(1)},\Gamma]^{[3]} + [\eta^{(2)}, W]^{[3]} + [\eta^{(3)},\Gamma]^{[3]} + [\eta^{(1)}, W]^{[4]} + [\eta^{(3)}, f]^{[4]} + [\eta^{(3)}, W]^{[4]}$$

$$\dot{W}(s) = [\eta^{(3)}, f]^{[2]} + [\eta^{(2)},\Gamma]^{[2]} + [\eta^{(2)}, W]^{[3]} + [\eta^{(3)},\Gamma]^{[3]} + [\eta^{(1)}, W]^{[4]} + [\eta^{(3)}, f]^{[4]}$$

- IM-SRG(2): 3rd-order exact for GS energy and 2nd-order exact for V_{eff}.
- IM-SRG(3): 4th-order exact for GS energy and 3rd-order exact for V_{eff}.
- IM-SRG is controlled and improvable method

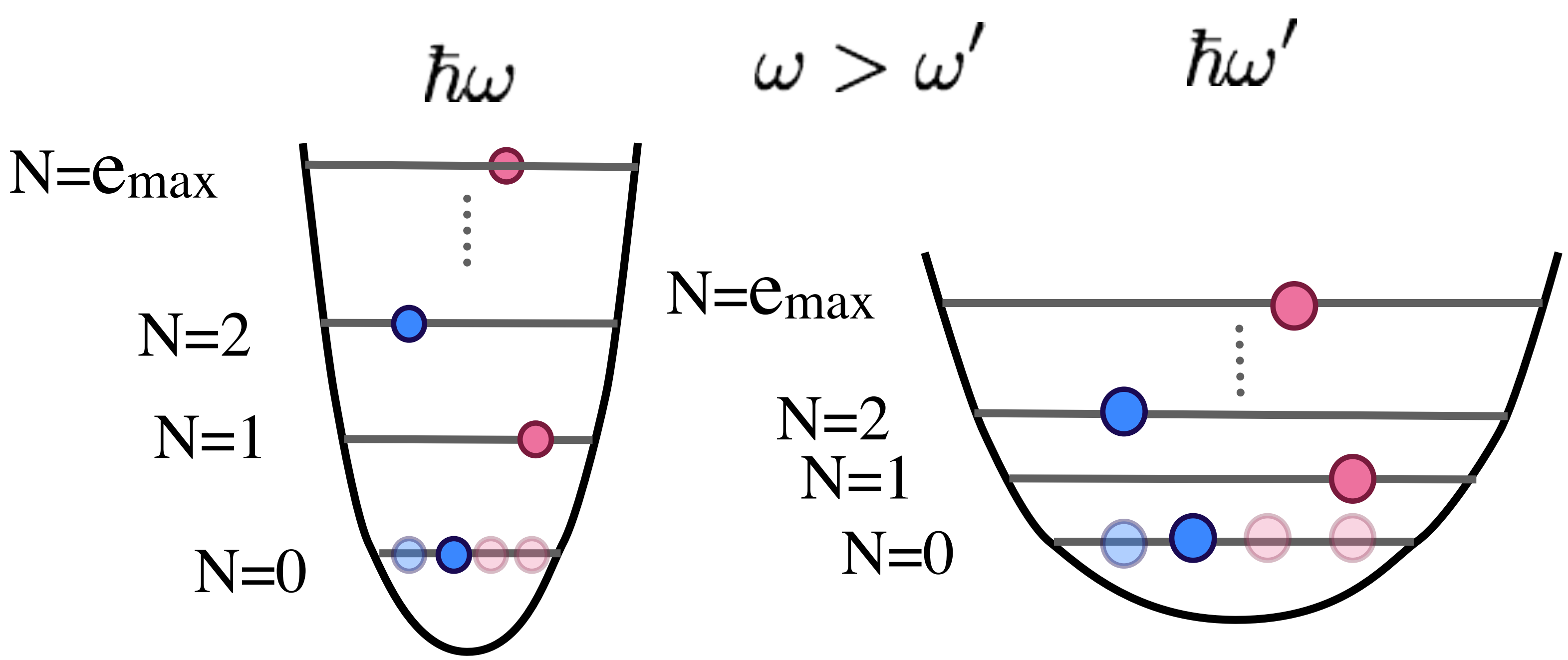
Numerical calculations

$$H(0) = T_{\rm rel} + V_{\rm NN} + \cancel{V_{\rm 3N} + V_{\rm 4N} + \cdots}$$

N^{3}LO (Λ=500MeV) from χEFT Entem-Machleidt, PRC **68**, 041001(R) (2003)

Free-space SRG evolved version $V_{\rm srg}$ (λ) Bogner-Perry-Furnstahl, PRC**75**, 061001 (2008)

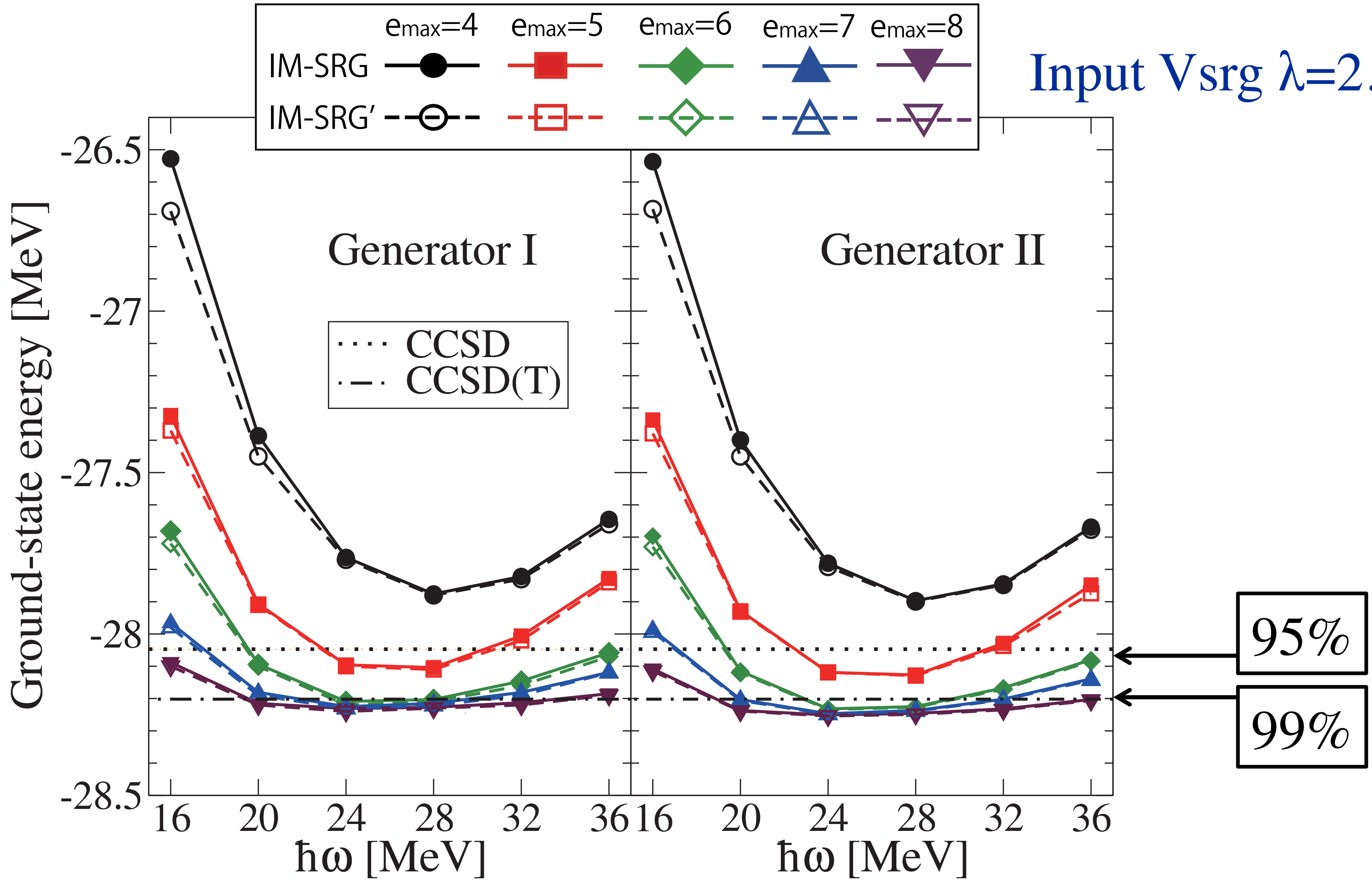
$$\boxed{\frac{d}{ds}\boldsymbol{f}(s) = \beta(\boldsymbol{f}, s)}$$



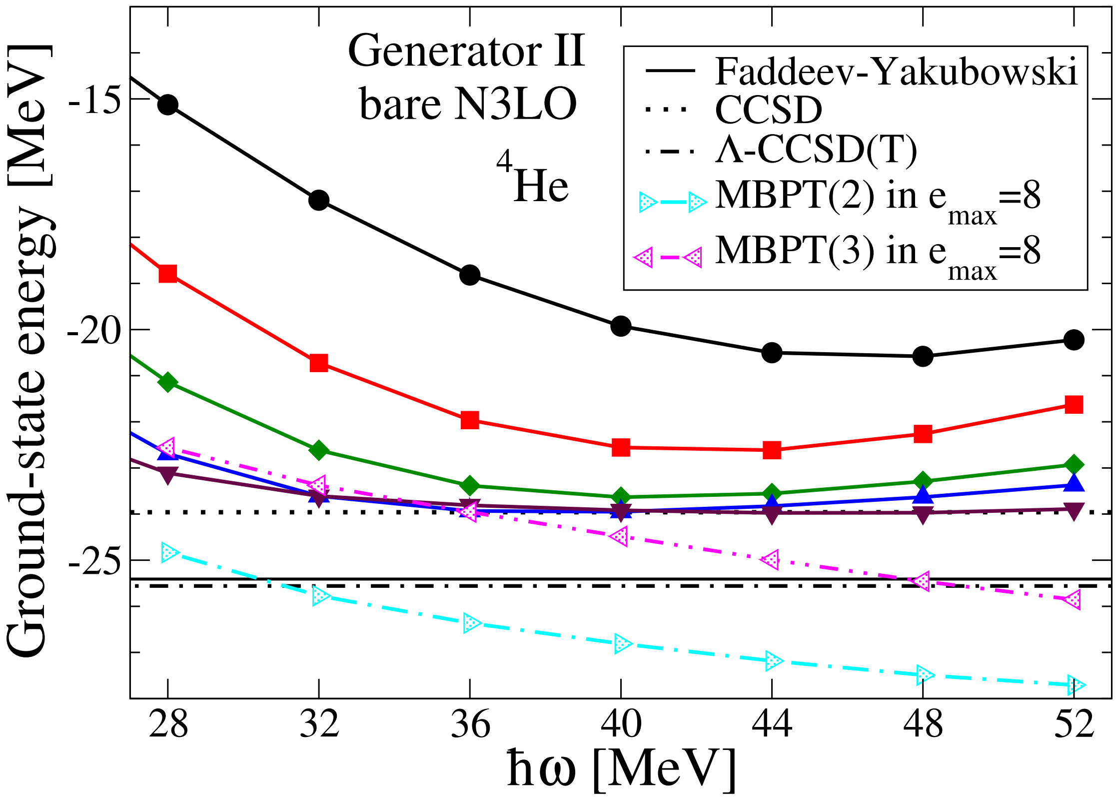
e_{max}	# SP	dim (f)
4	*30*	*3.4×10⁴*
5	*42*	*1.5×10⁵*
6	*56*	*4.7×10⁵*
7	*72*	*1.4×10⁶*
8	*90*	*3.5×10⁶*
10	*130*	*2.0×10⁷*

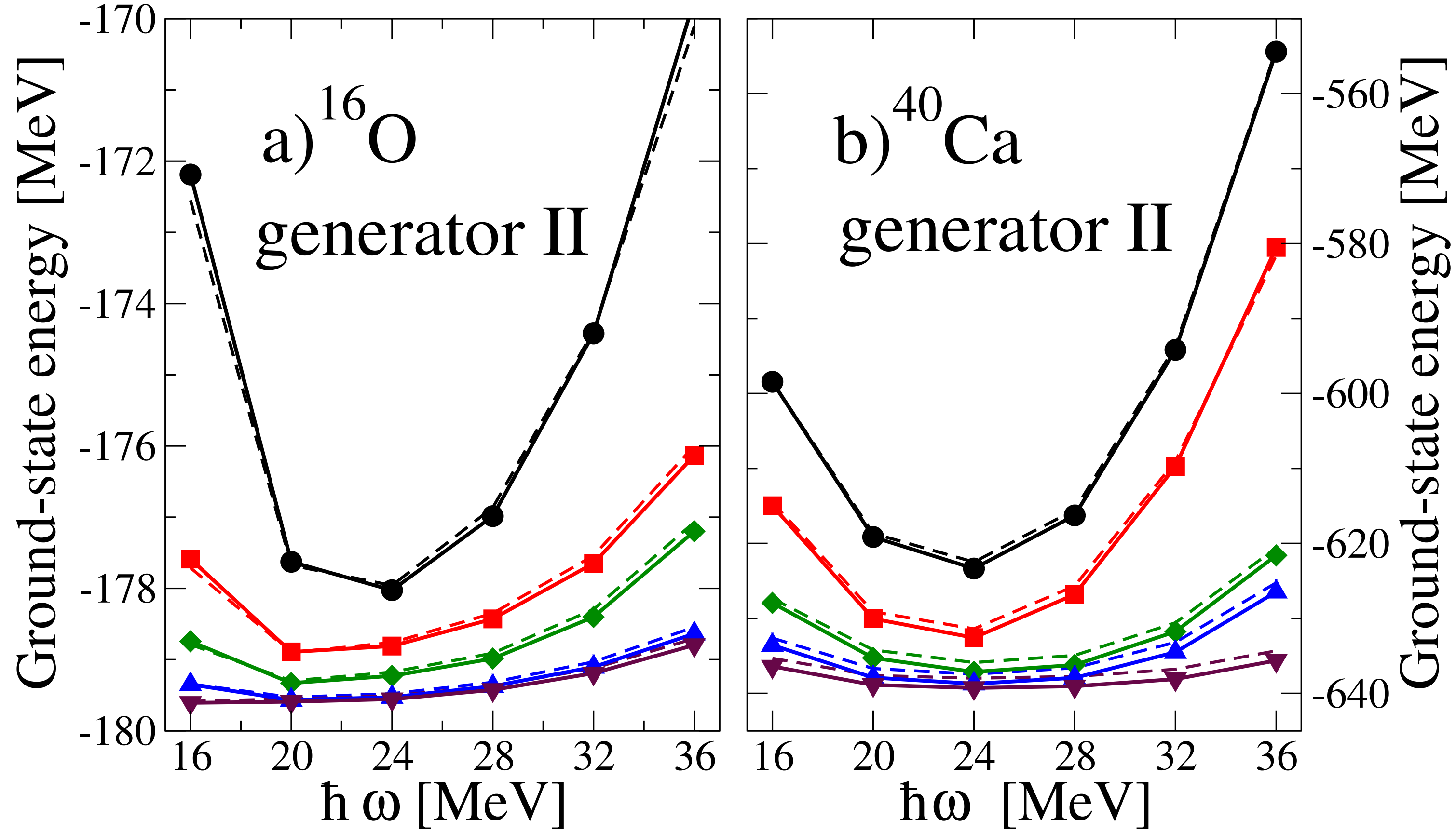
^{4}He with two different generators

Input Vsrg λ=2.0fm^{-1}

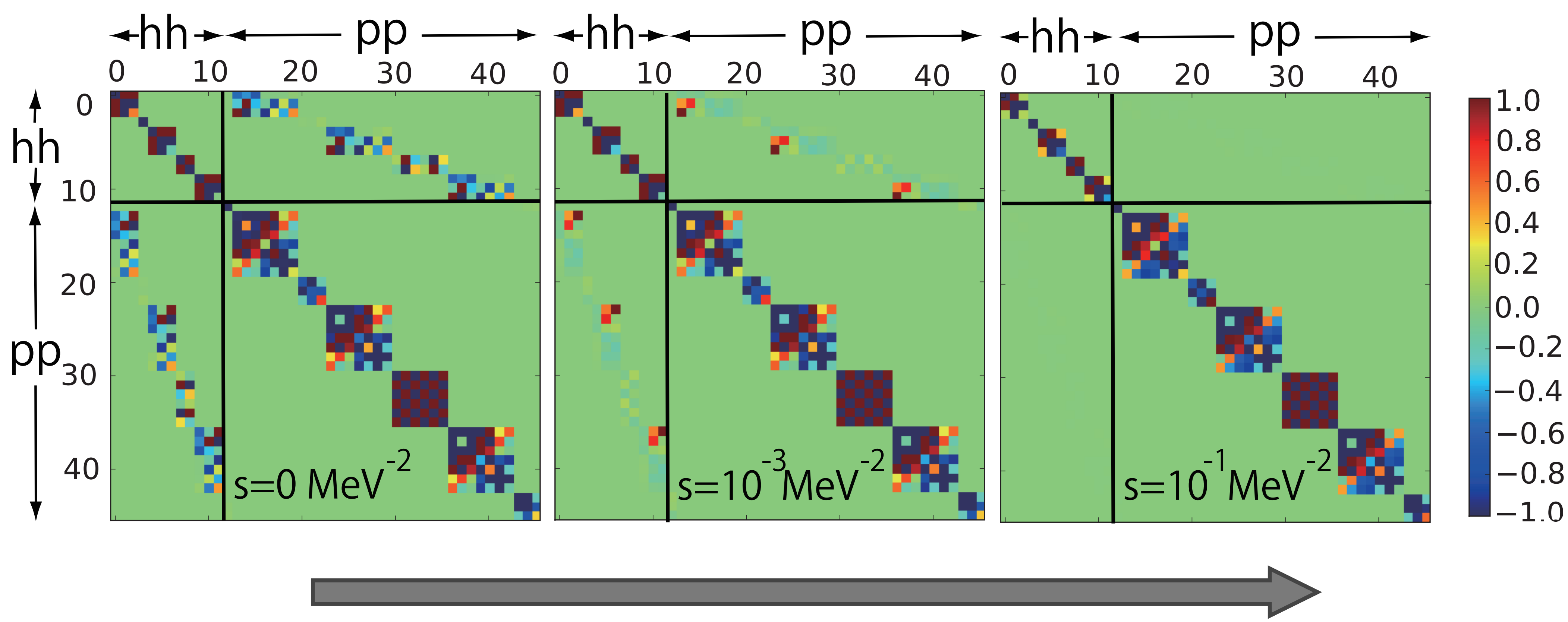


- Truncation up to normal-ordered 2-body level is a good approximation.





- Agrees well with CCSD (95% of correlation)
- MBPT(2,3) break down
- IM-SRG(2) work for ^{16}O and ^{40}Ca



H^{od} gets suppressed.

Evolution of operators

Arbitrary operator evolved on equal footing

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

$$\frac{d}{ds}\mathcal{O}_r(s) = [\eta, \mathcal{O}_r(s)] \qquad \mathcal{O}_r(s) = \mathcal{O}_r^{(0)}(s) + \mathcal{O}_r^{(1)}(s) + \mathcal{O}_r^{(2)}(s)\cdots$$

E.g., RMS radius

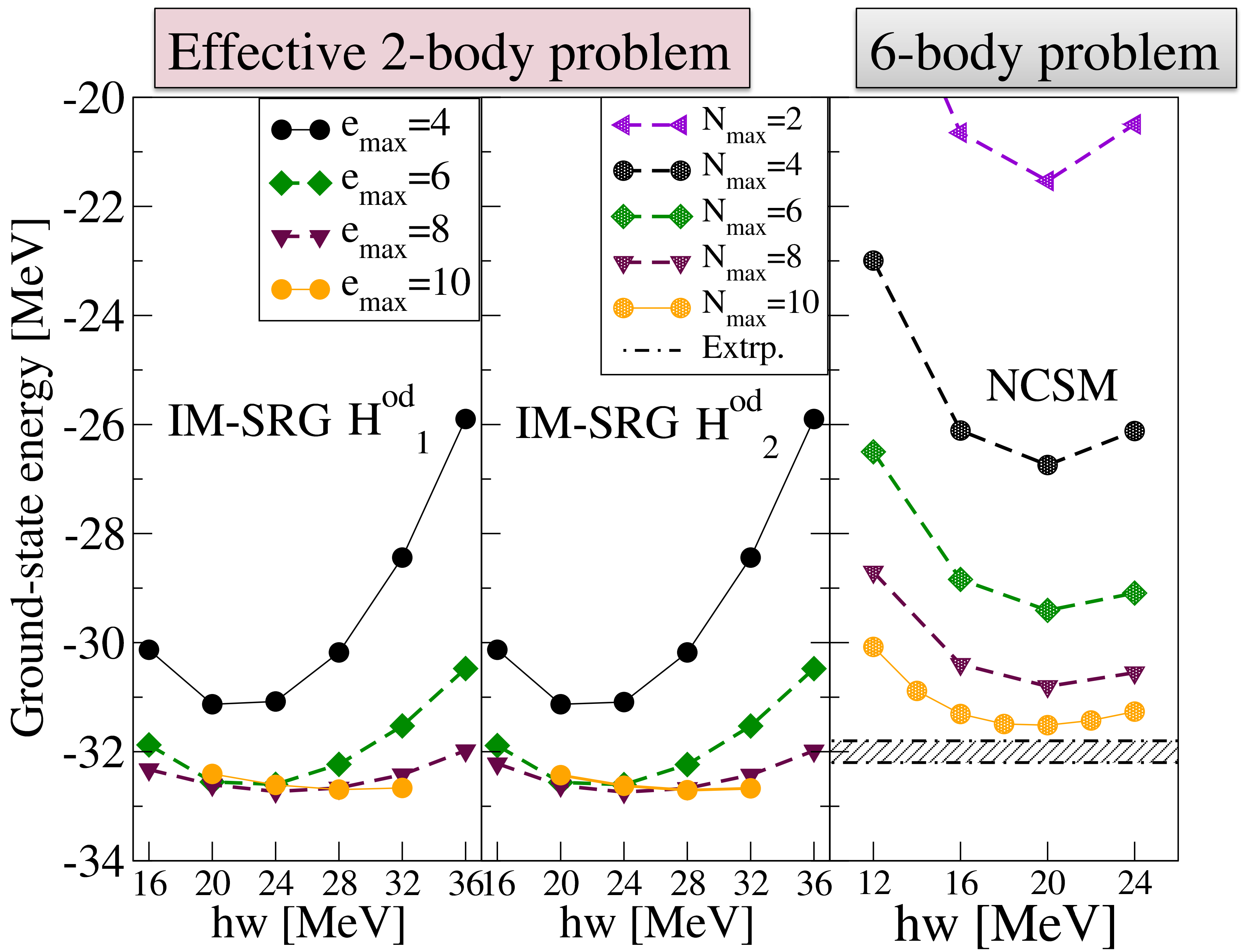
$$\mathcal{O}_r(0) \equiv \frac{1}{A}\sum_i (\vec{r}_i - \vec{R}_{\mathrm{cm}})^2$$

$$\langle r\rangle = \sqrt{\langle\psi|\,\mathcal{O}_r(0)\,|\psi\rangle} = \lim_{s\to\infty}\sqrt{\mathcal{O}_r^{(0)}(s)}$$

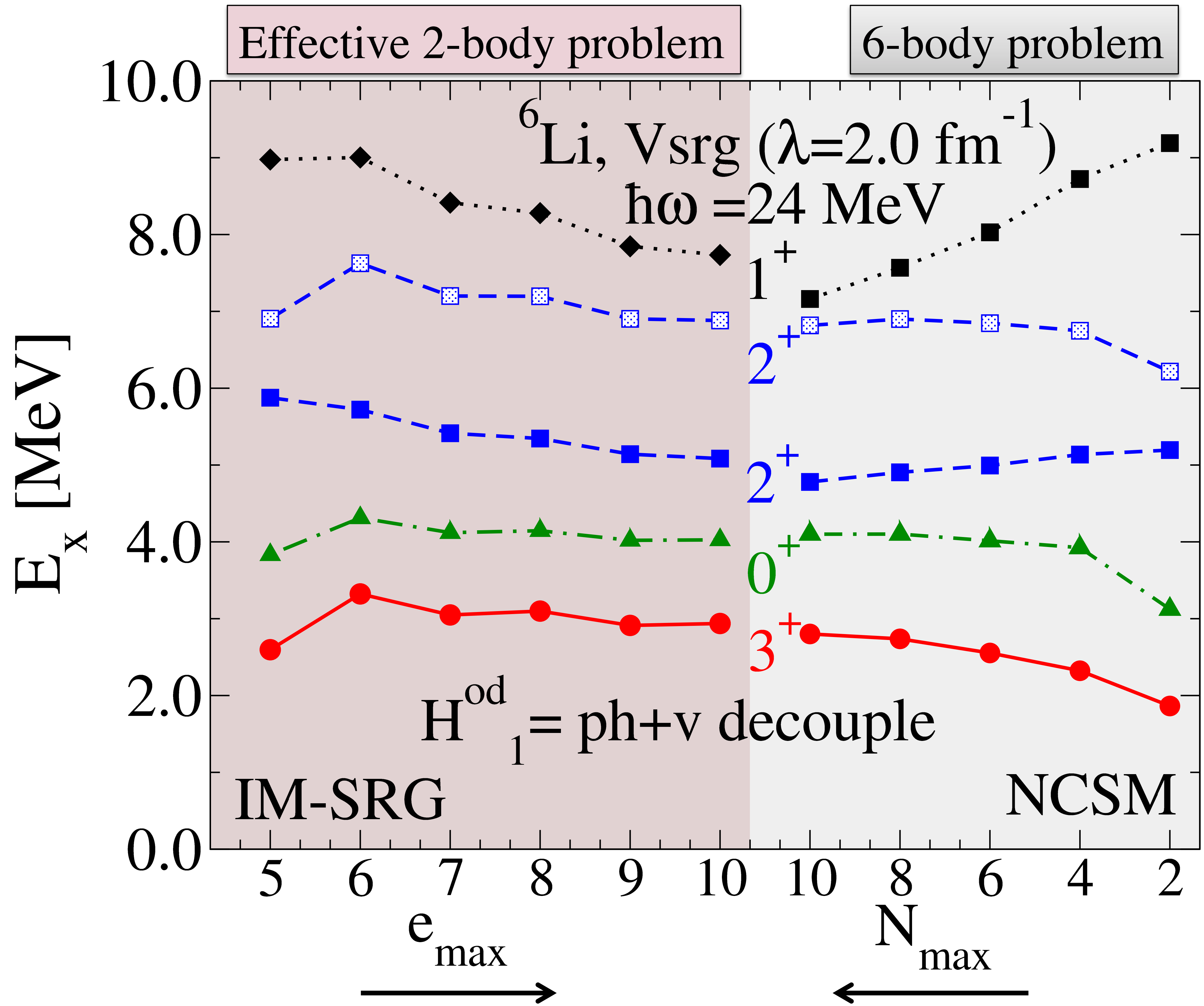
Joint benchmark is ongoing (NCFC, IT-NCSM,CCM,MBGF,UMOA,IM-SRG)
Results agree within uncertainty

Next step from H. Kamada et al., PRC64:044001(2001)

Ground-state convergence in ^{6}Li (^{4}He+"2" vs 6)



^{6}Li Spectra: IM-SRG vs NCSM



Works for 18-body as well

Summary

Summary

- ☑ We introduced SRG evolution of Hamiltonian in many-body medium (IM-SRG).
- ☑ We numerically demonstrated the features of in-medium SRG.
- ☑ Decoupling of a Hamiltonian, Size-extensivity, Non-perturbative feature.
- ☑ Radius (arbitral operators can be evolved).
- ☑ Contamination of center of mass excitation is very small.
- ☑ Shell-model effective interactions for valence nucleons (*p* and *sd*).

Work in Progress

- ☐ Derivation of effective operator.
- ☐ Systematic improvement; 3-body flow equations.