

In-medium similarity renormalization group for nuclei and nuclear matter

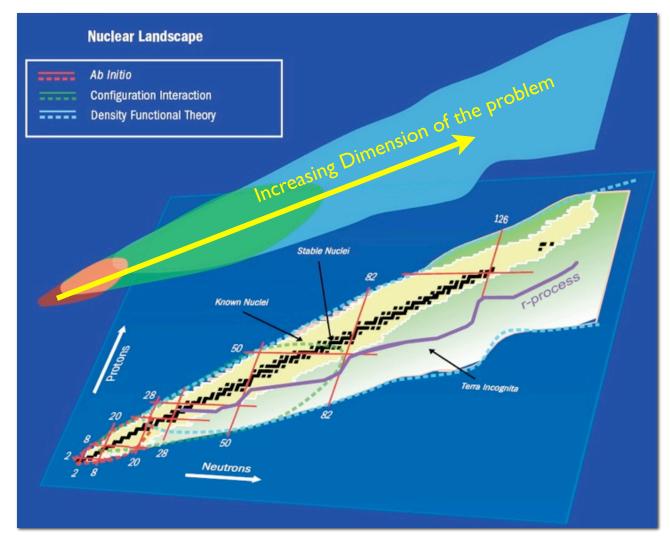
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*In collaboration with K.Tsukiyama (Tokyo) and A. Schwenk (Darmstadt)

The nuclear many-body landscape

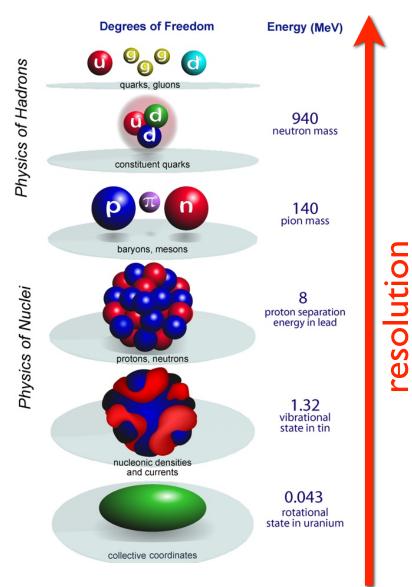


Calculate the properties of thousands of stronglyinteracting nuclei rooted in the underlying QCD

The nuclear many-body landscape **Nuclear Landscape** Challenges: 1) Extend the reach of ab-initio 2) next-generation energy density functionals 3) role of three-nucleon (and higher?) interactions 4) controlled theory of shell model Hamiltonians/operators

Calculate the properties of thousands of stronglyinteracting nuclei rooted in the underlying QCD

Multiple Scales in Nuclear Physics



Old View

- Multiple scales complicate life
- No easy way to connect them

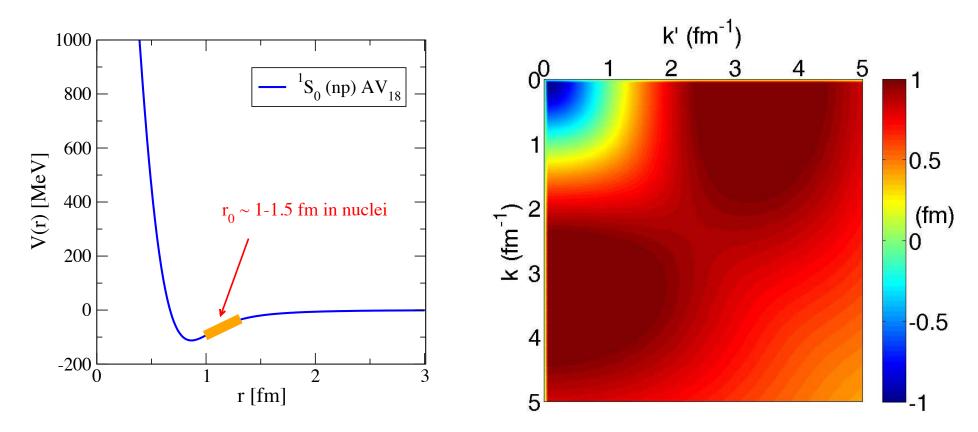
Modern View

- Ratio of scales => small parameters!
- Effective theories at each scale connected by renormalization group

 $V(\Lambda) = V_{2N}(\Lambda) + V_{3N}(\Lambda) + \cdots$

Use RG to pick a convenient Λ

Scale-dependent sources of non-perturbative physics



Repulsive core & strong tensor force => low and high k modes strongly coupled by the interaction

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

Example: Why large Λ 's are painful

Assume we want to compute the binding energy of a nucleus with mass number A in a wave function based approach. Assume that the interaction has a momentum cutoff Λ .

Q: What are the minimum requirements for the model space?

- A:
- The basis must be sufficiently extended in position space to capture a nucleus with radius R≈1.2 A[%] fm
- 2. The basis must be sufficiently extended in momentum space to capture the cutoff Λ .
- THUS: we need approximately K=(RΛ/(2π))³ single-particle states (phase space volume!) In practice K≈(RΛ/2)³ ~ Λ³A.

Computation of oxygen: $\Lambda=4/\text{fm}$ and $R\approx2.5\text{fm}$ Thus, our model space has about $K=5^3 = 125$ single-particle states. Matrix dimension: $D=K!/(K-A)!/A! \approx (K/A)^A \approx 8^{16} \approx 2^{48} \approx 10^{14}$.

Thus, the matrix dimension is D=K!/((K-A)! A!), with K≈(RA/2)³ ³

Example: Why large Λ 's are painful

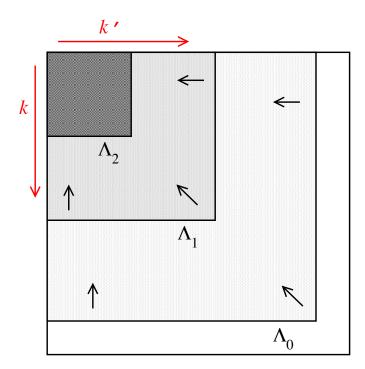
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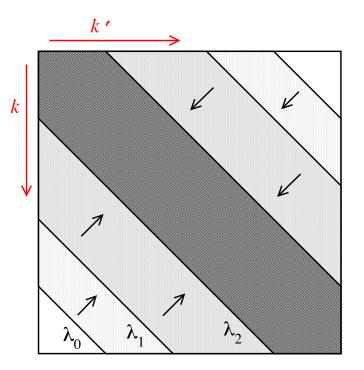
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Easiest way to extend the reach of ab-initio to heavier nuclei is to use lower resolutions (Λ) "physical" scales k_F and m_{π} ~ 1 fm⁻¹...

2 Types of Renormalization Group Transformations



"V_{low k}" integrate-out high k states preserves observables for $k < \Lambda$



"Similarity RG" eliminate far off-diagonal coupling preserves "all" observables

Very similar consequences despite differences in appearance (low and high momentum decoupled)

The Similarity Renormalization Group

Wegner, Glazek and Wilson

Unitary transformation via flow equations:

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

Engineer η to do different things as $\lambda \Rightarrow 0$

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

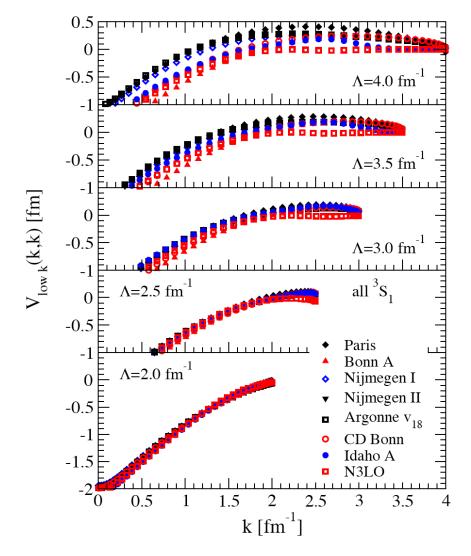
 $\eta(\lambda) = [\mathcal{G}_{\lambda}, H_{\lambda}]$

 $\mathcal{G}_{\lambda} = T \implies H_{\lambda} \text{ driven towards diagonal in } \mathbf{k} - \text{space}$ $\mathcal{G}_{\lambda} = PH_{\lambda}P + QH_{\lambda}Q \implies H_{\lambda} \text{ driven to block-diagonal}$ \vdots

•

Good things happen at lower resolution scales!

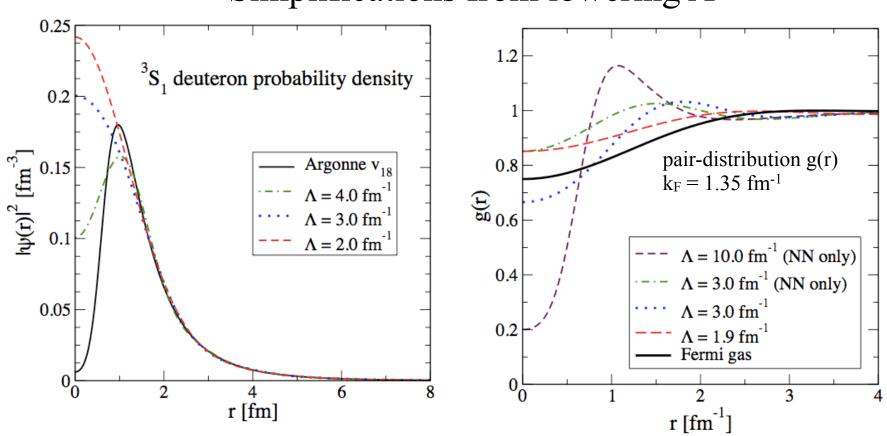
Example: universal low-momentum nuclear Hamiltonian



All nuclear force models have the same long-distance structure...

...but are totally modeldependent at short-distances

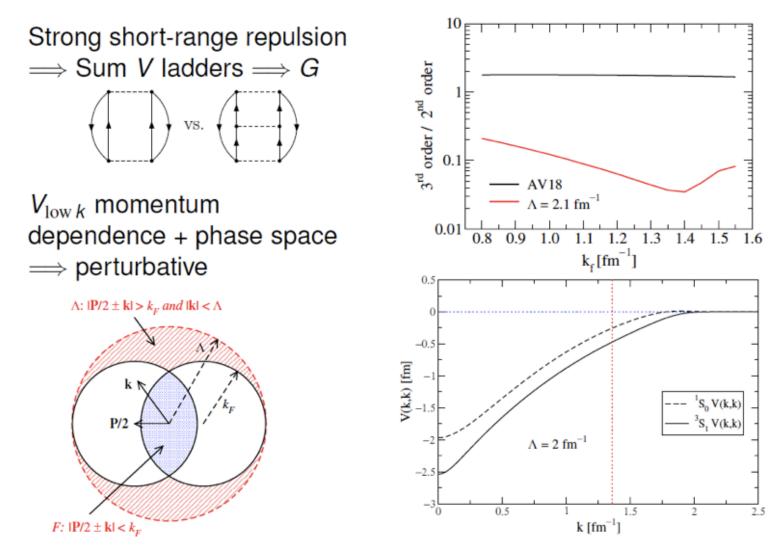
Under RG evolution, the different models "collapse" to a universal curve



Simplifications from lowering Λ

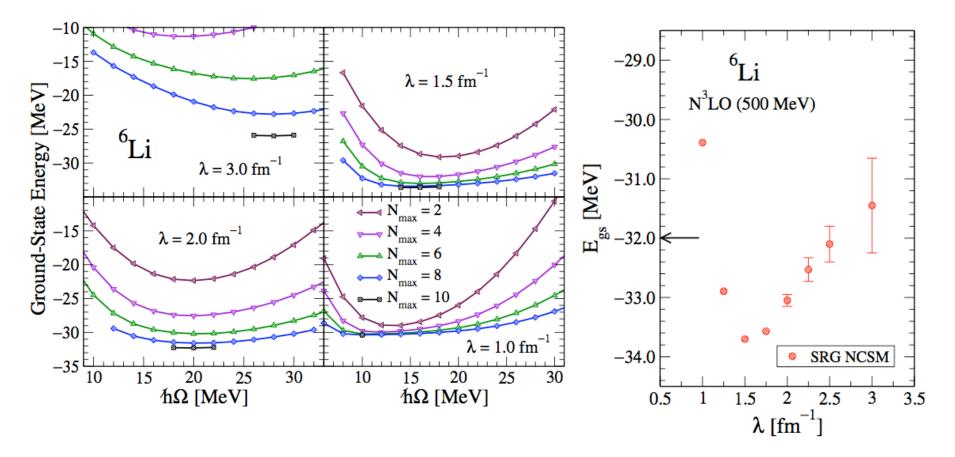
correlations in wave functions blurred out more effective variational calcs., efficient basis expansions, more perturbative...

Lowering Λ increases "perturbativeness"



"nuclear matter" calculations relevant for neutron stars, nuclear equation of state, etc. become perturbative

Full Configuration Interaction (FCI) Calculations

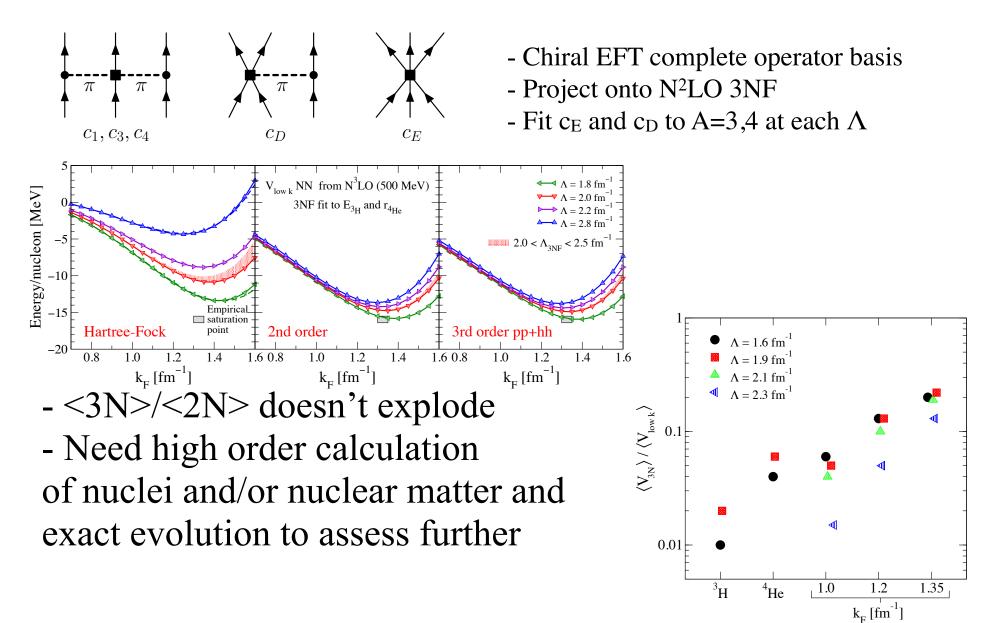


Decoupling high-k and low-k => accelerated convergence, more perturbative

BUT note...

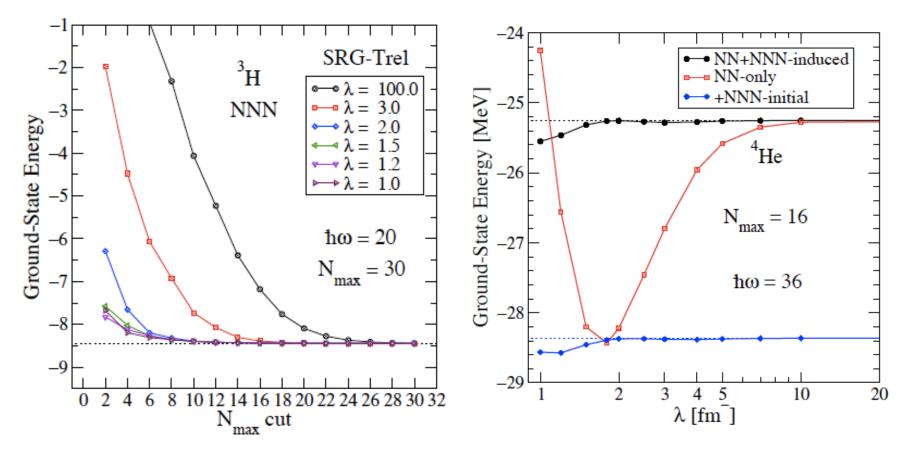
 λ -dependent results (omitted induced 3...A-body forces)

Approximation to the full 3N evolution



Consistent 3N SRG evolution

(Jurgenson, Navratil, Furnstahl)



It works! λ -independent ³H, softer convergence Induced 4N are small (but see R. Roth's talk for possible problems)

Free space versus in-medium evolution

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

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

Use T + V(λ)_{2N} + V(λ)_{3N} + ... + V(λ)_{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 normalordering

Normal Ordered Hamiltonians

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

$$\begin{aligned} A_i A_j A_k A_l \cdots A_m &= N(A_i A_j A_k A_l \cdots A_m) \\ &+ N \left((\overrightarrow{A_i A_j A_k A_l} \cdots A_m) + \text{all other single contractions} \right) \\ &+ N \left((\overrightarrow{A_i A_j A_k A_l} \cdots A_m) + \text{all other double contractions} \right) \\ &\vdots \end{aligned}$$

+
$$N\left(\left(\text{all fully contracted terms}\right)\right)$$

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

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

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

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

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

$$E_{vac} = \langle \Phi | H | \Phi \rangle$$

$$f_i = t_{ii} + \sum_h \langle ih | V_2 | ih \rangle n_h + \frac{1}{2} \sum_{hh'} \langle ihh' | V_3 | ihh' \rangle n_h n_{h'}$$

$$\Gamma_{ijkl} = \langle ij | V_2 | kl \rangle + \sum_h \langle ijh | V_3 | klh \rangle n_h$$

$$W_{ijklmn} = \langle ijk | V_3 | lmn \rangle \qquad \langle \Phi | N(\cdots) | \Phi \rangle = 0$$

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

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In-medium SRG for Nuclear matter

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

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

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

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

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

$$\langle 12 | \Gamma_{od} | 34 \rangle = 0 \text{ if } f_{12} = f_{34}$$

- Truncate to 2-body normal-ordered operators "IM-SRG(2)"
 - dominant parts of induced many-body forces included implicitly

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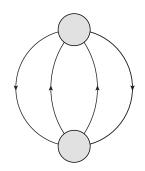
$$H(\infty) = E_{vac}(\infty) + \sum f_i(\infty)N(a_i^{\dagger}a_i) + \frac{1}{4}\sum [\Gamma_d(\infty)]_{ijkl}N(a_i^{\dagger}a_j^{\dagger}a_la_k)$$

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

In-medium SRG Equations Infinite Matter

O-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

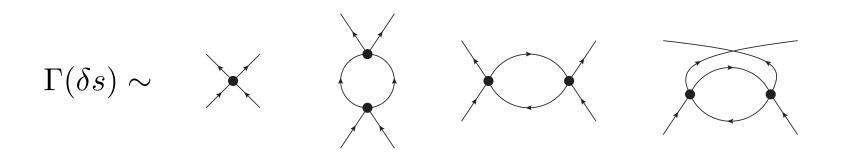
In-medium SRG Equations Infinite Matter

2-body flow

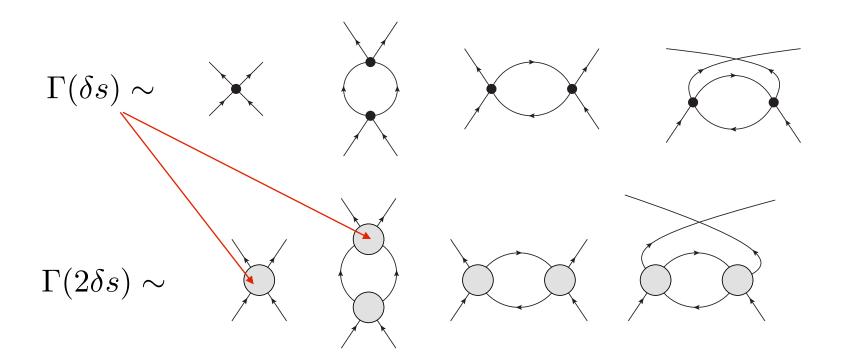
$$\langle 12 | \frac{d\Gamma}{ds} | 34 \rangle = -(f_{12} - f_{34})^2 \langle 12 | \Gamma | 34 \rangle + \frac{1}{2} \sum_{ab} (f_{12} + f_{34} - 2f_{ab}) \langle 12 | \Gamma | ab \rangle \langle ab | \Gamma | 34 \rangle (1 - n_a - n_b) + \sum_{ab} [(f_{1a} - f_{3b}) - (f_{2b} - f_{4a})] \langle 1a |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

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

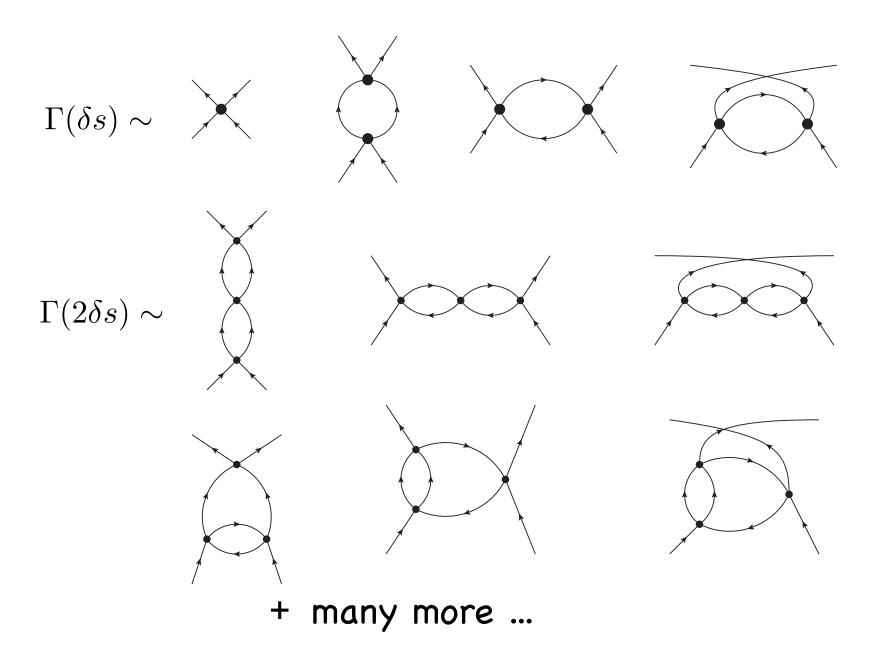
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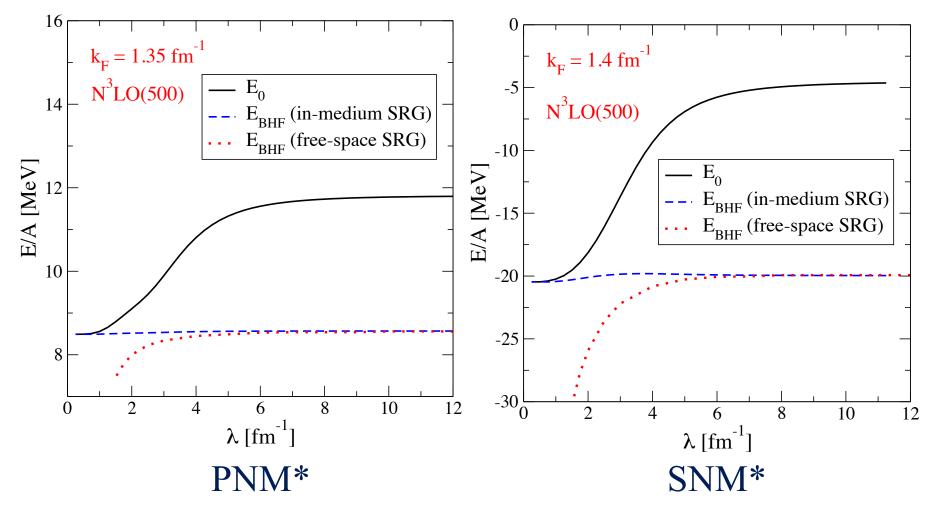
Some observations

1)
$$\frac{d}{ds}\langle H
angle_0 \leq 0$$
 for monotonic f_k

correlations weakened, HF picks up more binding with increasing s.

- 2) pp channel + 2 ph channels treated on equal footing
- 3) Intrinsically non-perturbative
- 4) no unlinked diagrams (size extensive, etc.)
- 5) "3rd-order exact" a-la CCSD
- 6) Extension to effective operators/Shell model possible

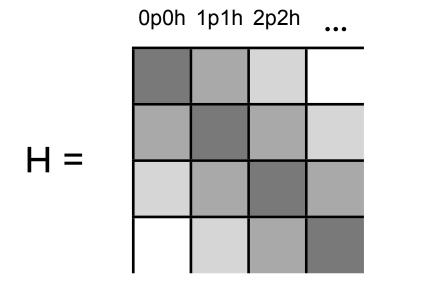
Correlations "adiabatically" summed into $H(\lambda)$



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.)



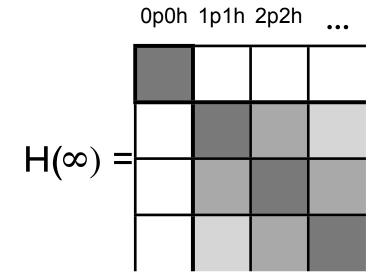
Df. "offdiagonal" part of H as terms that mix 0p0h with higher ph sectors

$$\eta(s) = [H(s), H^{od}(s)]$$

$$\Gamma^{od} = \sum_{pp'hh'} \Gamma_{pp'hh'} N(a_p^{\dagger} a_{p'}^{\dagger} a_h a_{h'}) + h.c$$

$$f^{od} = \sum_{ph} f_{ph} N(a_p^{\dagger} a_h) + h.c.$$

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



HF reference state decouples from higher npnh states

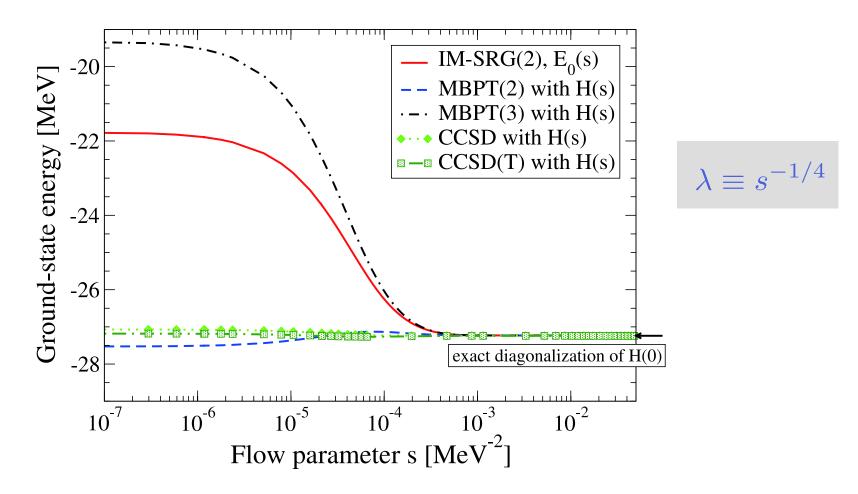
$$\lim_{s \to \infty} \langle \phi | H(s) | \phi \rangle = E_{gs}$$

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

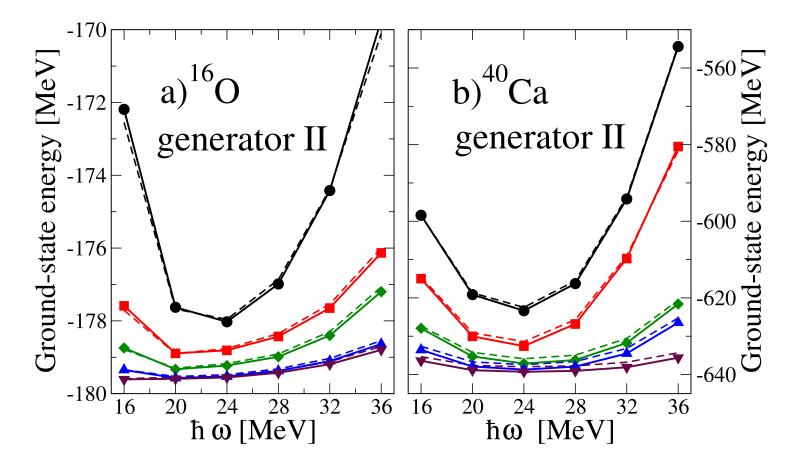
$$QH(\infty)P = 0, \quad PH(\infty)Q = 0,$$

where $P = |\Phi\rangle \langle \Phi|$ and $Q = 1 - P.$

IM-SRG to build "soft" interactions

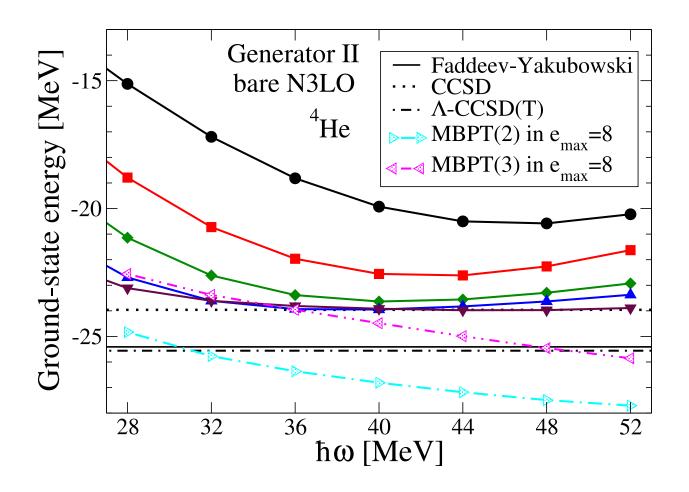


 $\sim \lambda$ -independent CC results (dominant induced many-body interactions included)



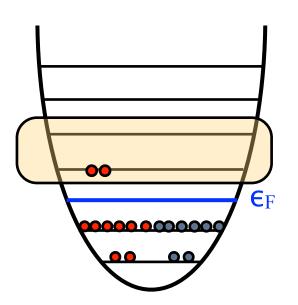
- good agreement with CCSD (dashed lines)
- N⁶ scaling with number of s.p. orbitals

Also works well for harder interactions:



- agrees well w/CCSD using bare N³LO (Entem/Machleidt)

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



inactive particle orbitals q_i

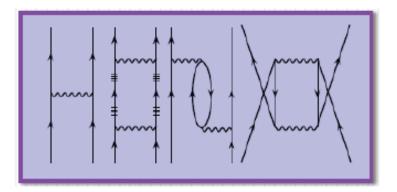
active valence orbitals v_i

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

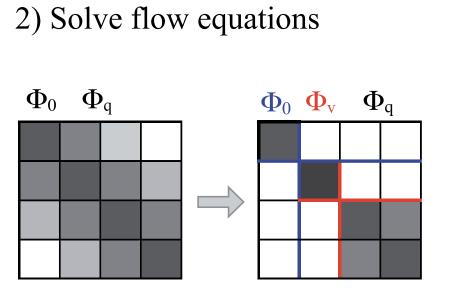


Can we use the IM-SRG to do this?

In-medium SRG recipe for shell model

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

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



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

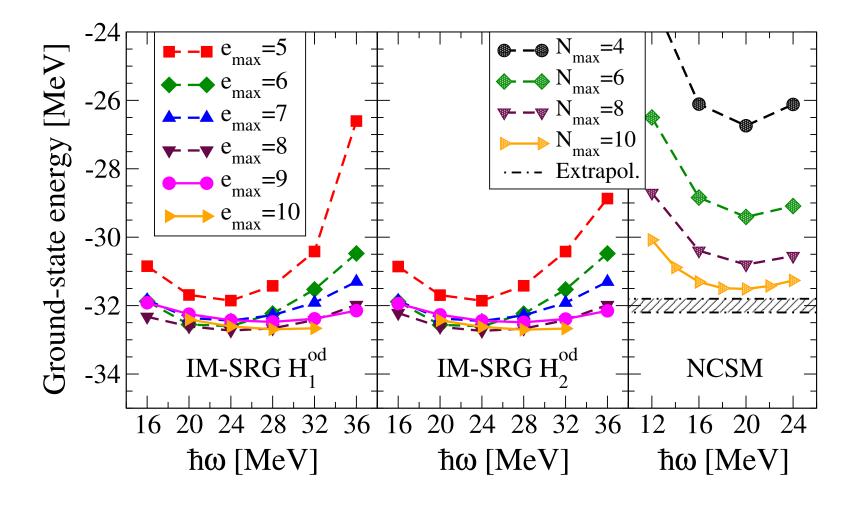
$$\eta = [H^{(od)}, H]$$

$$H^{(od)} = \sum g_i \hat{O}_i$$

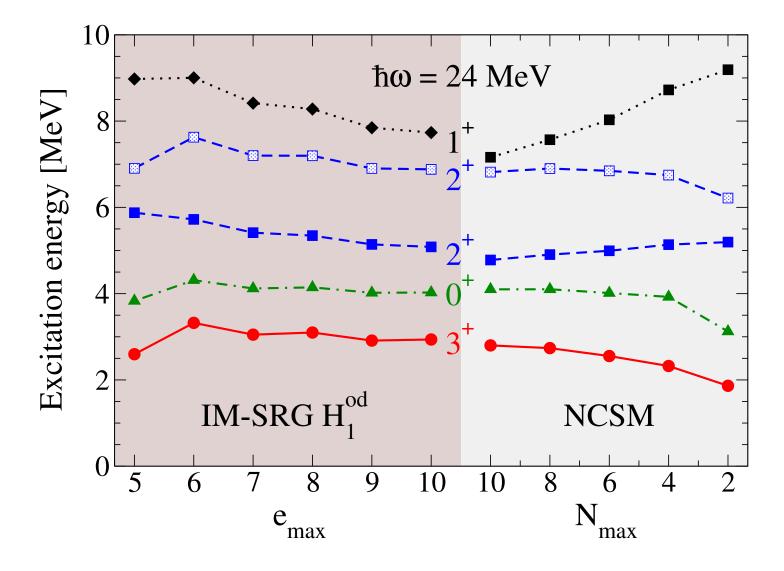
3) Diagonalize fully-evolved H in the reduced valence space

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

⁶Li ground state: comparison to exact NCSM



⁶Li 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 normalordering => 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

Ongoing work

I) Extension to open-shell nuclei using number-projected HFB reference states (Heiko Hergert, Ohio State)

II) Extension to shell model effective operators (e.g., $0\nu\beta\beta$ decay) - suitable for multi-shell model spaces and non-perturbative

III) Apply to neutron/nuclear matter in a box

IV) Next higher truncation (explicit N-ordered 3-body)