

In-medium Similarity Renormalization Group for nuclei

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Essential Points

I. Similarity renormalization group (SRG)

II. SRG transformation in many-body medium

- ❖ Decoupling of ground states
- ❖ Non perturbativeness
- ❖ Size-extensivity
- ❖ (Potential applicability to $V_{\text{eff}}/O_{\text{eff}}$)

Nuclei From Scratch

Description of nuclei from nucleonic degrees of freedom (ab initio).

- ▶ Binding-energy systematics
- ▶ Low-lying excitations and spectroscopy
- ▶ Collective excitations with Large- or small amplitude
- ▶ Phenomena at the extreme conditions (T, J, N/Z ...)

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Tremendous progress has been made over the past decade

- Green's Function Monte Carlo (A=12)
- No-core Shell Model (A=14)
- Coupled-Cluster/ Unitary Model Operator Approach (near closed shell)
- Green's function method (quasi particle structure around closed shell)

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One obstacle to extending such calculations to heavier nuclei

=> Strong coupling between low- and high-momentum states induced by the short-distance details of typical two- and three-nucleon interactions, from low-energy scattering data and deuteron.

Understanding nuclei from RG perspective

Nuclear Hamiltonian is "resolution" dependent

$$H(\Lambda) = T + V^{(2)}(\Lambda) + V^{(3)}(\Lambda) \dots$$

Relevant details of high-energy physics \Rightarrow Λ -dependent coefficients of operators in a low-energy Hamiltonian.

Decoupling of high momentum d.o.f. can be achieved by lowering the "resolution scale", or Λ , down to typical nuclear structure momentum scale. \Rightarrow Necessary d.o.f. for low-energy observables.

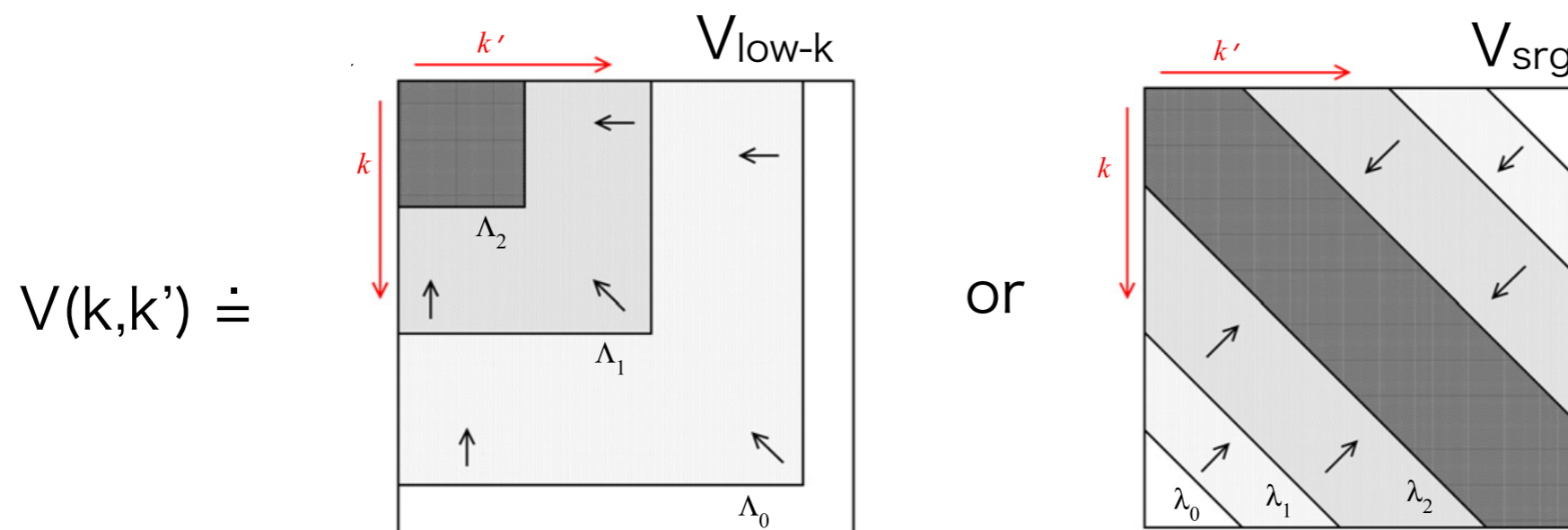
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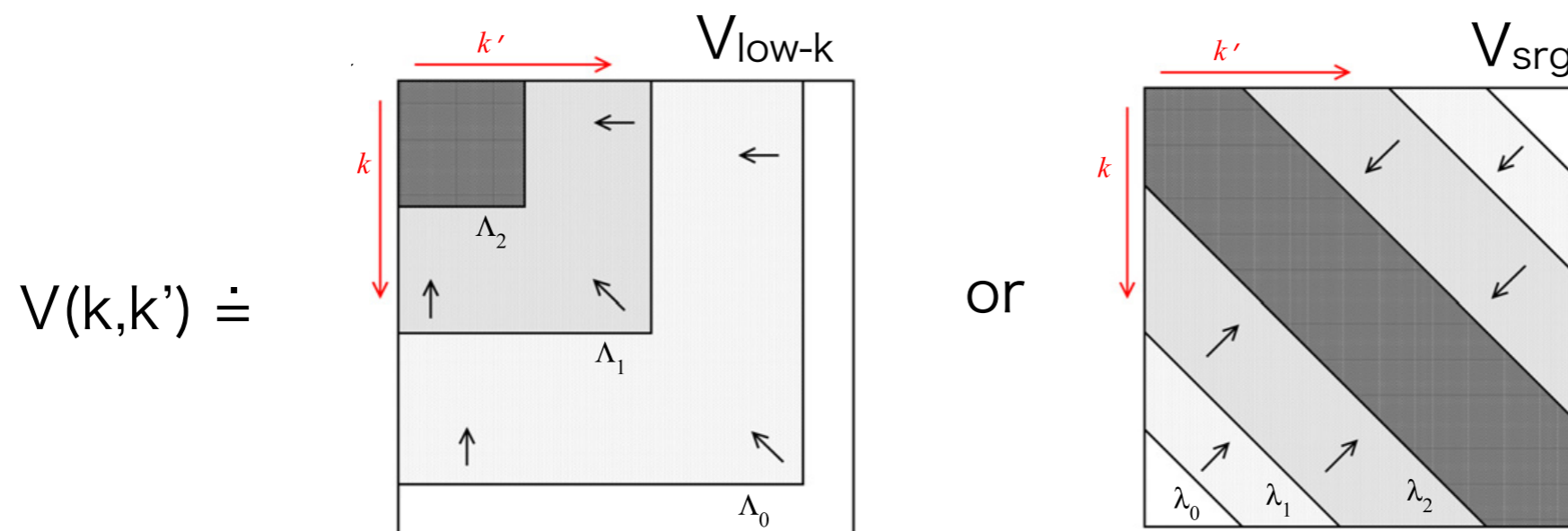
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◆ Greatly simplify the nuclear many-body problems, making those calculations **converge rapidly**.

◆ Varying Λ provides a powerful tool to assess **theoretical errors** due to truncation in Hamiltonian and many-body approximations.

Similarity Renormalization Group

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

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powerful alternative to Lee-Suzuki

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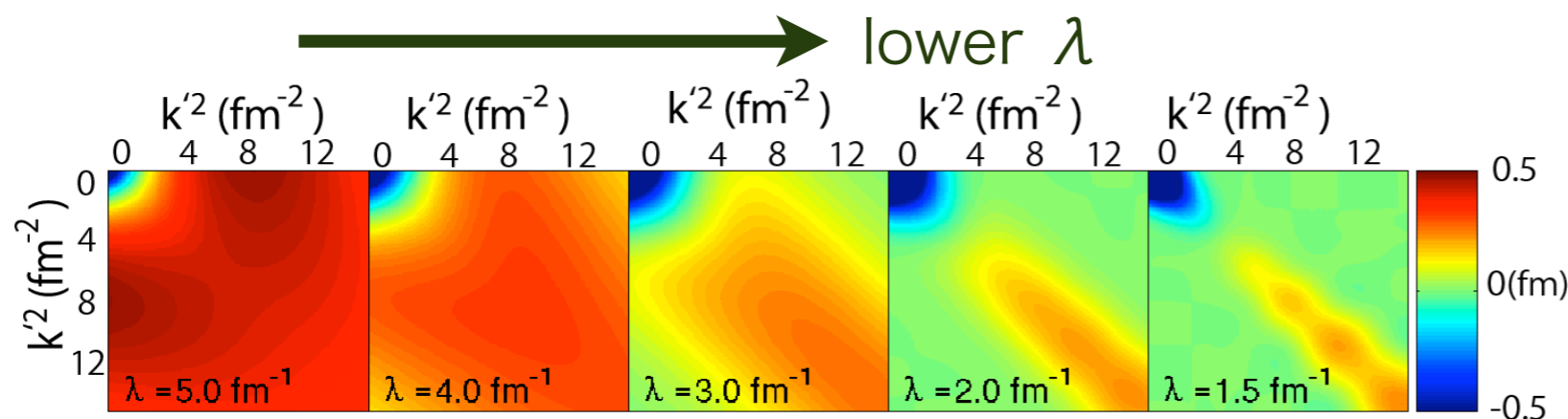
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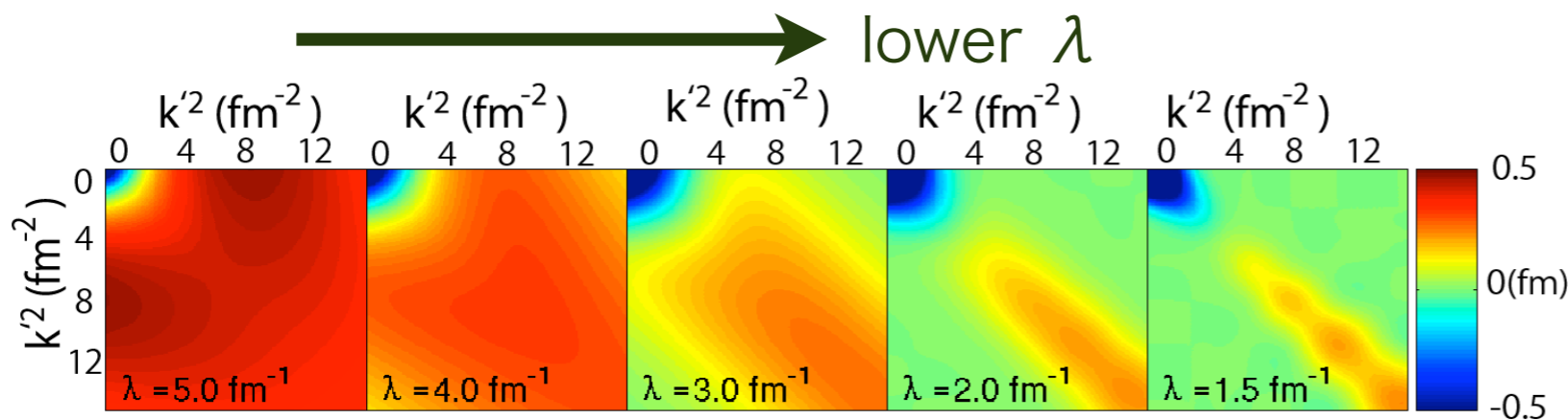
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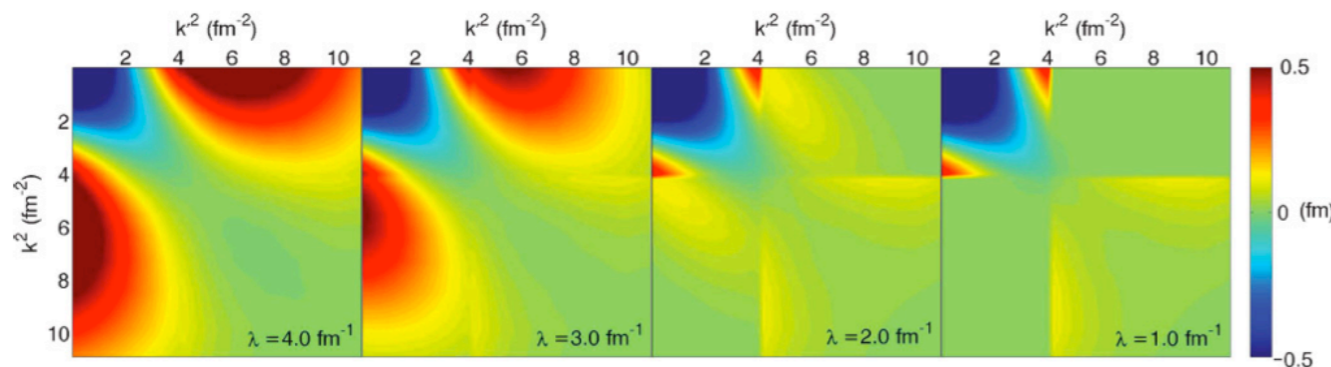
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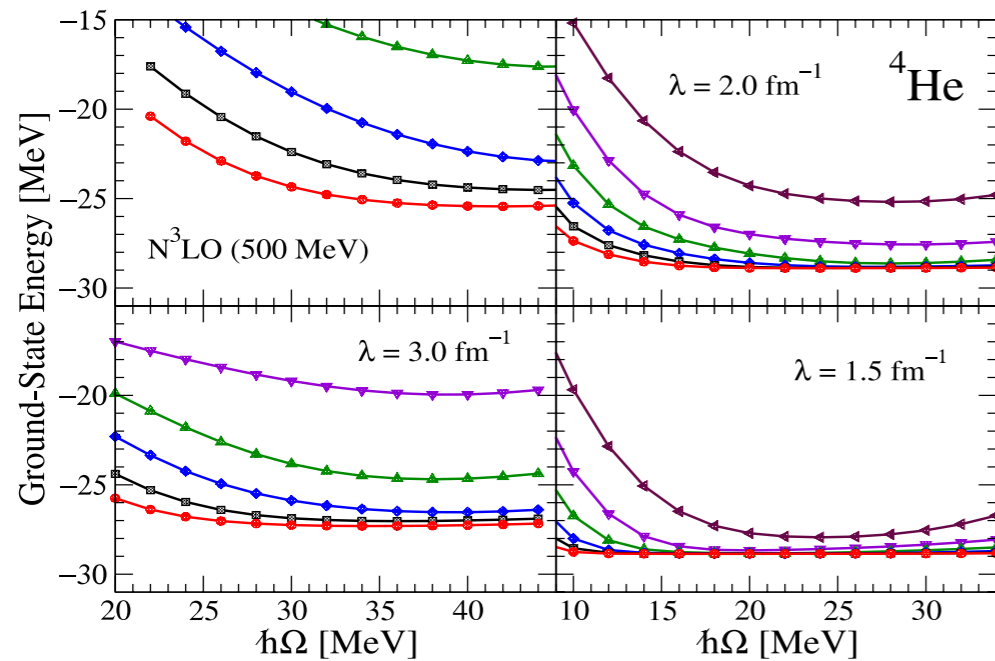


$$H^d(s) = \begin{pmatrix} PH(s)P & 0 \\ 0 & QH(s)Q \end{pmatrix}$$

Anderson et al, PRC77, 037001 (2008)

RG and many-body interactions

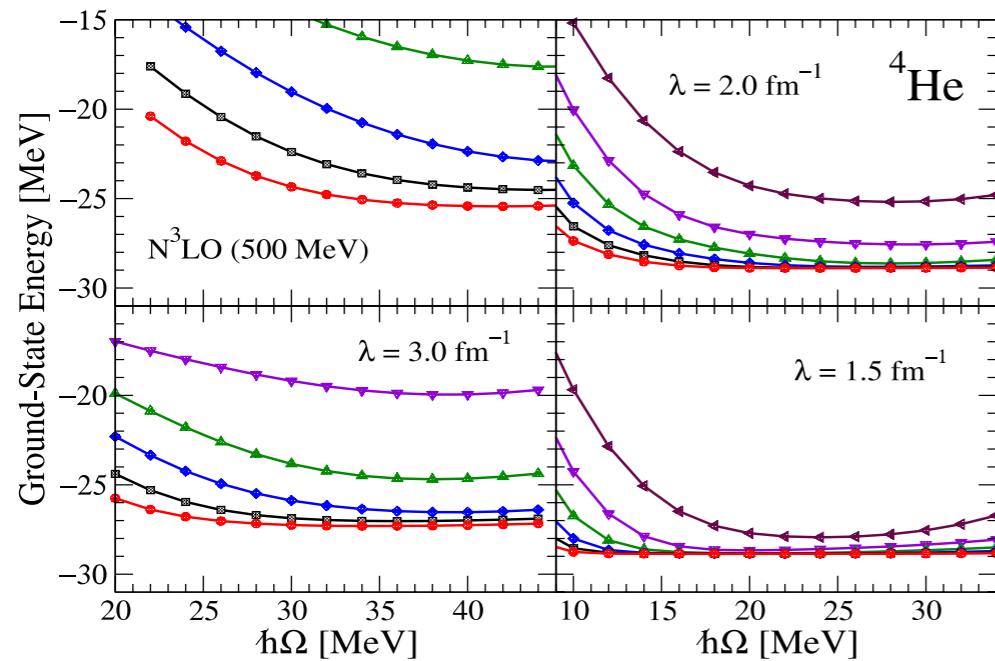
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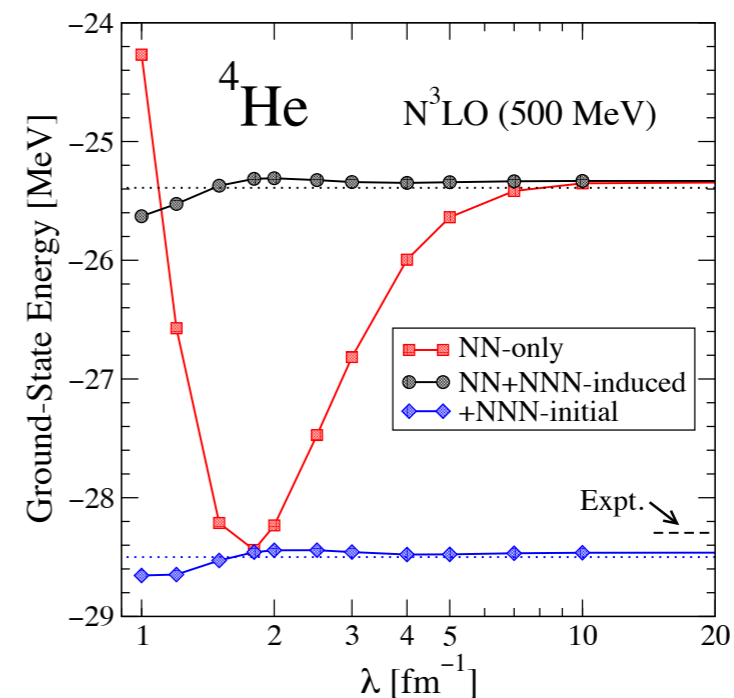
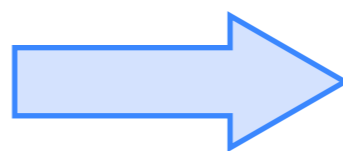
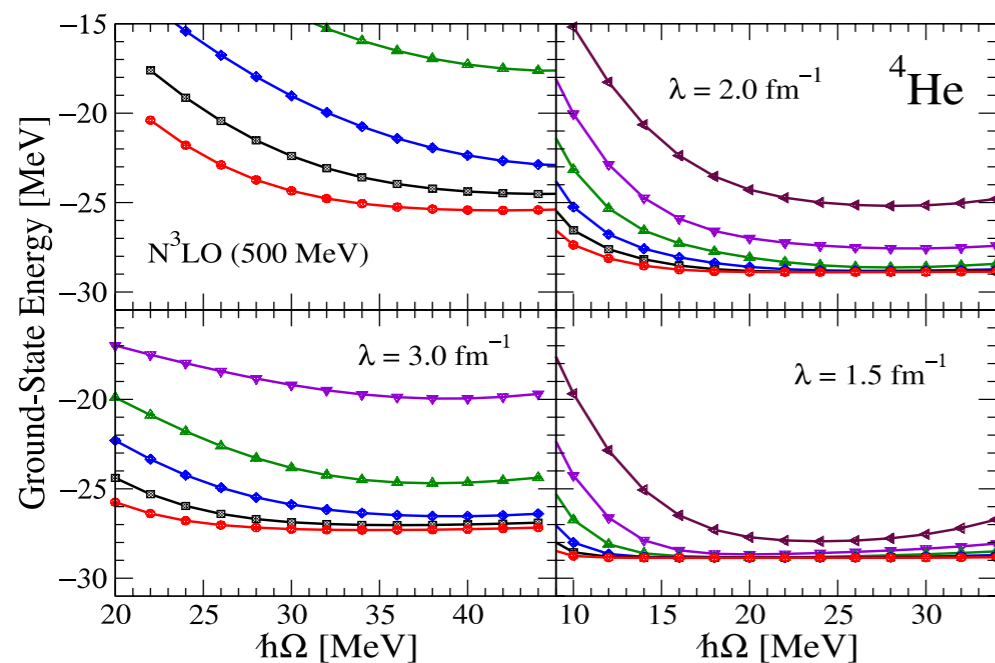
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Many-body forces are induced and do affect observables

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

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Jurgeson, Furnstahl and Navratil Phys Rev. Lett. 103, 082501(2009)

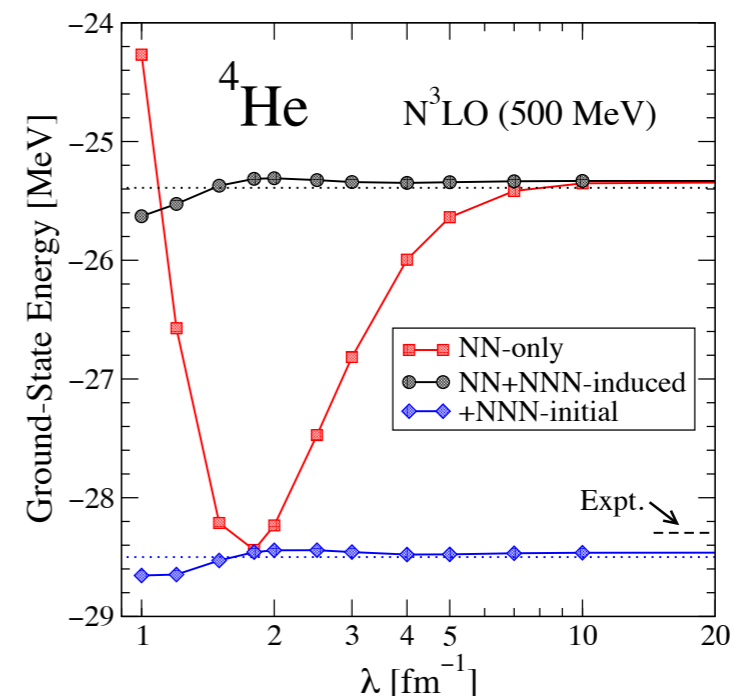
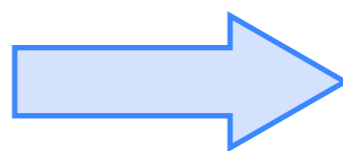
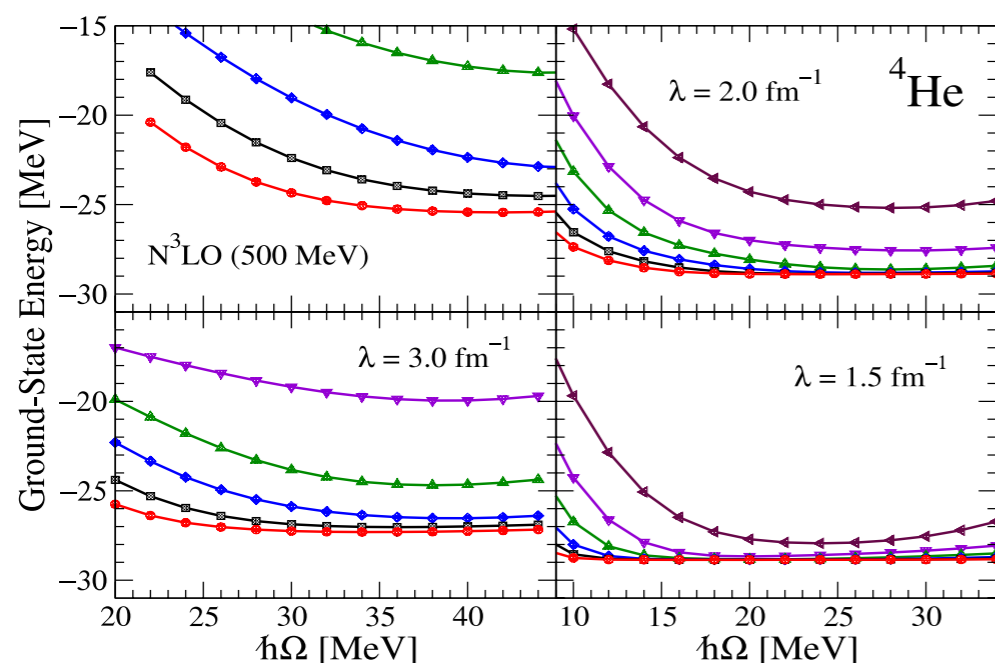
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SRG transformation directly **in many-body system**

- ✳ Normal-ordering w.r.t. a reference state, and truncate at a finite order.
- ✳ One can approximately evolve 3-body, ..A-body operators within 2b machinery.

K.T. S. Bogner and A. Schwenk, to be submitted

In-medium SRG for Nuclei

Starting with a general Hamiltonian

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

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All operators can be normal-ordered wrt a finite-density Fermi vacuum $|\Phi\rangle$

$$\hat{H} = E_0 + \sum_{kk'} g_{kk'} \{a_k^\dagger a'_k\} + \frac{1}{2!^2} \sum_{kpqr} \Gamma_{kpqr} \{a_k^\dagger a_p^\dagger a_r a_q\} + \frac{1}{3!^2} \sum_{kpqrst} W_{kpqrst} \{a_k^\dagger a_p^\dagger a_q^\dagger a_t a_s a_r\},$$

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$$\Gamma_{pqrs} = V_{pqrs}^{(2)} + \frac{1}{4} \sum_i V_{pqirsi}^{(3)} n_i.$$

$$n_i \equiv \theta(\epsilon_F - \epsilon_i)$$

zero- one- two-body terms include contributions from 3N, 4N.. forces

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Truncating the flow equation up to normal-ordered 2-body operators may approximately evolve induced 3-body and higher-body interactions through density- dependent coefficients.

What we drive a Hamiltonian toward

We define what is suppressed in the flow

$$H^{od}(s) = f^{od}(s) + \Gamma^{od}(s)$$

$$\begin{cases} \Gamma^{od}(s) &= \sum_{pp'hh'} \Gamma_{pp'hh'}(s) \{a_p^\dagger a_{p'}^\dagger a_h a_{h'}\} + h.c. \\ f^{od}(s) &= \sum_{ph} f_{ph}(s) \{a_p^\dagger a_h\} + h.c. \end{cases}$$

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$$\eta^I = [H^d, H] \longrightarrow \frac{d}{ds} \text{Tr}(H^{od}(s))^2 = -2\text{Tr}(\eta^\dagger \eta) \leq 0$$

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White's choice [J. Chem. Phys, 117, 7472 \(2002\)](#)

$$\eta^{II} = \sum_{ph} \frac{f_{ph}}{f_p - f_h - \Gamma_{phph}} \{a_p^\dagger a_h\} - h.c. + \sum_{pp'hh'} \frac{\Gamma_{pp'hh'}}{f_p + f_{p'} - f_h - f_{h'} + A_{pp'hh'}} \{a_p^\dagger a_{p'}^\dagger a_{h'} a_h\} - h.c.$$

monopole interaction
monopole interaction

$$A_{pp'hh'} = \Gamma_{pp'pp'} + \Gamma_{hh'hh'} - \Gamma_{phph} - \Gamma_{p'h'p'h'} - \Gamma_{ph'ph'} - \Gamma_{p'h'p'h}$$

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- Hamiltonians using η^I and η^{II} are unitary equivalent **if no truncation is made.**
- Any discrepancies in energy eigenvalues provides a **measure of the truncation errors** from the neglected 3-body or higher-body operators.

Decoupling of Hilbert space

Solving the flow equation for normal-ordered operators

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

builds up correlations in pp, hh and ph channels to all order in bare couplings

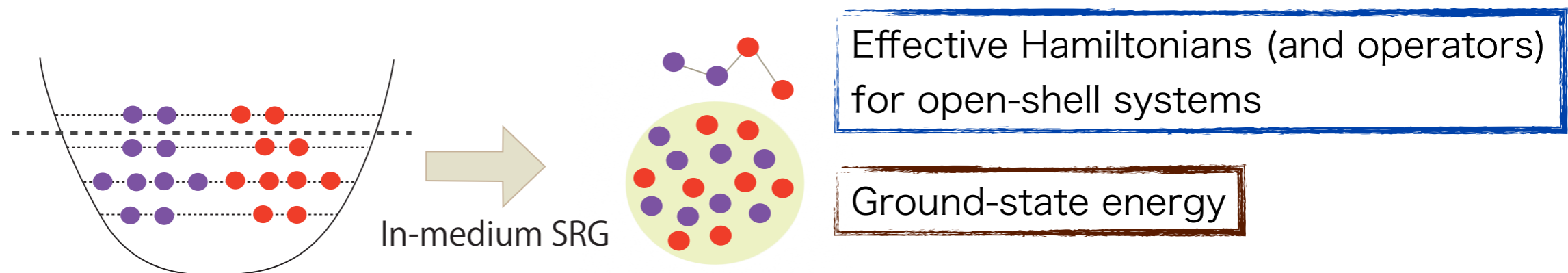
At the end of the flow

$$H(\infty) = E_0(\infty) + f^d(\infty) + \Gamma^d(\infty).$$

- The reference state $|\Phi\rangle$ becomes the ground state of $H(\infty)$ with $E_0(\infty)$
- The $|\Phi\rangle$ is decoupled from the rest of the Hilbert space

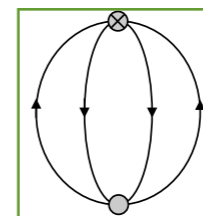
$$QH(\infty)P = 0, \quad PH(\infty)Q = 0$$

$$P = |\Phi\rangle\langle\Phi| \text{ and } Q = 1 - |\Phi\rangle\langle\Phi|$$



In-medium SRG(2) Flow Equation

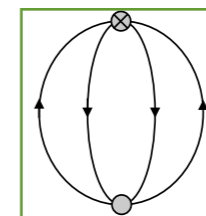
$$\frac{dE_0}{ds} = \sum_{ij} \eta_{ij}^{(1)} f_{ji}(n_i - n_j) + \frac{1}{2} \sum_{ijkl} \eta_{ijkl}^{(2)} \Gamma_{kl ij} n_i n_j \bar{n}_k \bar{n}_l \quad (\bar{n}_i \equiv 1 - n_i),$$



- The commutator form \implies no unlinked diagrams
 \implies **size-extensive**, with truncation errors scaling linearly with A .
- SRG is intrinsically **non-perturbative**.
- Modest scaling of computational efforts \implies suitable for medium-mass nuclei

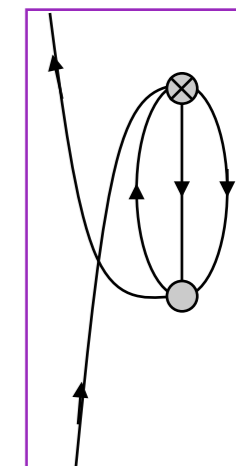
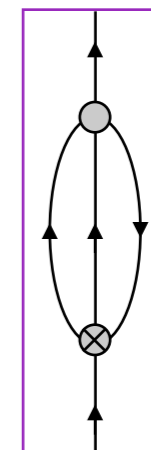
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$$\frac{df_{12}}{ds} = \sum_i \left\{ (\eta_{1i}^{(1)} f_{i2}) + (1 \leftrightarrow 2) \right\} + \sum_{ij} (n_i - n_j) (\eta_{ij}^{(1)} \Gamma_{j1 i2} - f_{ij} \eta_{j1 i2}^{(2)})$$

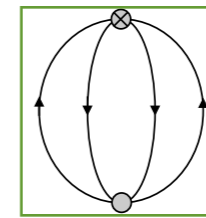
$$+ \frac{1}{2} \sum_{ijk} \left\{ \eta_{k1 ij}^{2b} \Gamma_{ijk2} (n_i n_j \bar{n}_k + \bar{n}_i \bar{n}_j n_k) + (1 \leftrightarrow 2) \right\},$$



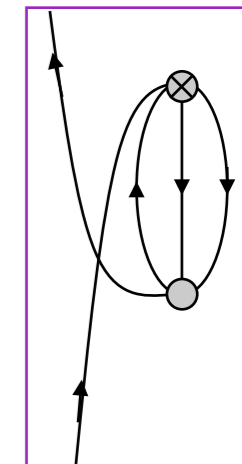
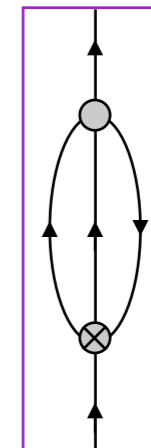
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 \implies **size-extensive**, with truncation errors scaling linearly with A.
- SRG is intrinsically **non-perturbative**.
- Modest scaling of computational efforts \implies suitable for medium-mass nuclei

In-medium SRG(2) Flow Equation

$$\frac{dE_0}{ds} = \sum_{ij} \eta_{ij}^{(1)} f_{ji} (n_i - n_j) + \frac{1}{2} \sum_{ijkl} \eta_{ijkl}^{(2)} \Gamma_{klij} n_i n_j \bar{n}_k \bar{n}_l \quad (\bar{n}_i \equiv 1 - n_i),$$



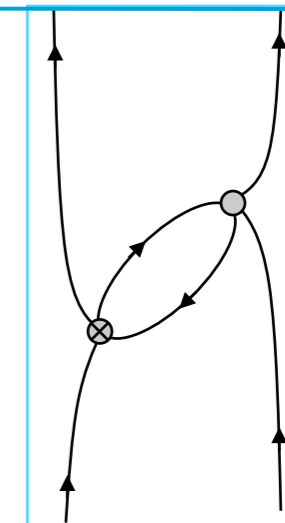
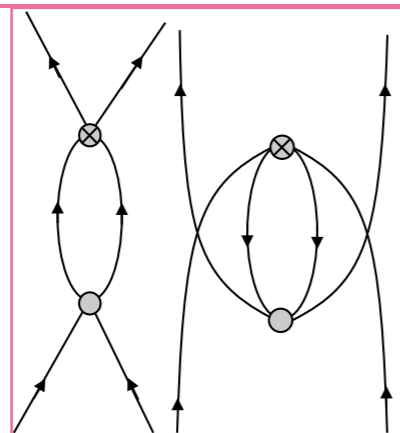
$$\frac{df_{12}}{ds} = \sum_i \left\{ (\eta_{1i}^{(1)} f_{i2}) + (1 \leftrightarrow 2) \right\} + \sum_{ij} (n_i - n_j) (\eta_{ij}^{(1)} \Gamma_{j1i2} - f_{ij} \eta_{j1i2}^{(2)})$$



$$+ \frac{1}{2} \sum_{ijk} \left\{ \eta_{k1ij}^{2b} \Gamma_{ijk2} (n_i n_j \bar{n}_k + \bar{n}_i \bar{n}_j n_k) + (1 \leftrightarrow 2) \right\},$$

$$\frac{d\Gamma_{1234}}{ds} = \sum_i \left\{ (\eta_{1i}^{(1)} \Gamma_{i234} - f_{1i} \eta_{i234}^{(2)}) - (1 \leftrightarrow 2) \right\} - \sum_i \left\{ (\eta_{i3}^{(1)} \Gamma_{12i4} - f_{i3} \eta_{12i4}^{(2)}) - (3 \leftrightarrow 4) \right\}$$

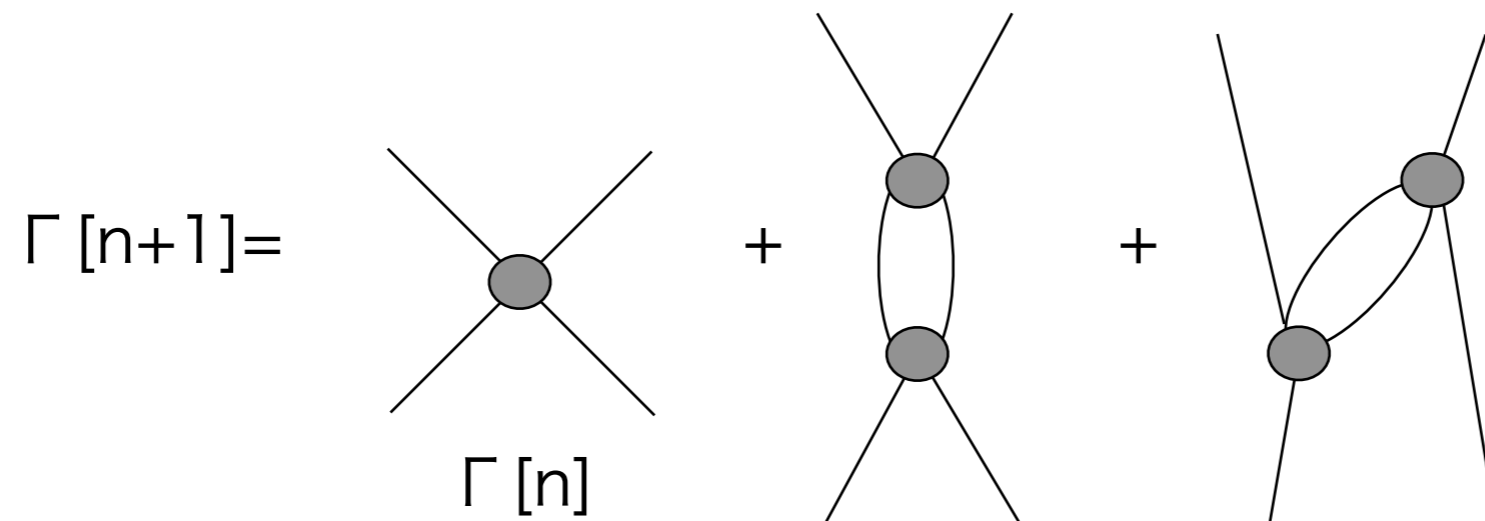
$$+ \frac{1}{2} \sum_{ij} \left\{ \eta_{12ij}^{(2)} \Gamma_{ij34} (\bar{n}_i \bar{n}_j - n_i n_j) + (1, 2 \leftrightarrow 3, 4) \right\} + \sum_{ij} (\bar{n}_i n_j - n_i \bar{n}_j) \left[\left\{ \eta_{j2i4}^{(2)} \Gamma_{i1j3} - \eta_{i1j3}^{(2)} \Gamma_{j2i4} \right\} - (1 \leftrightarrow 2) \right]$$



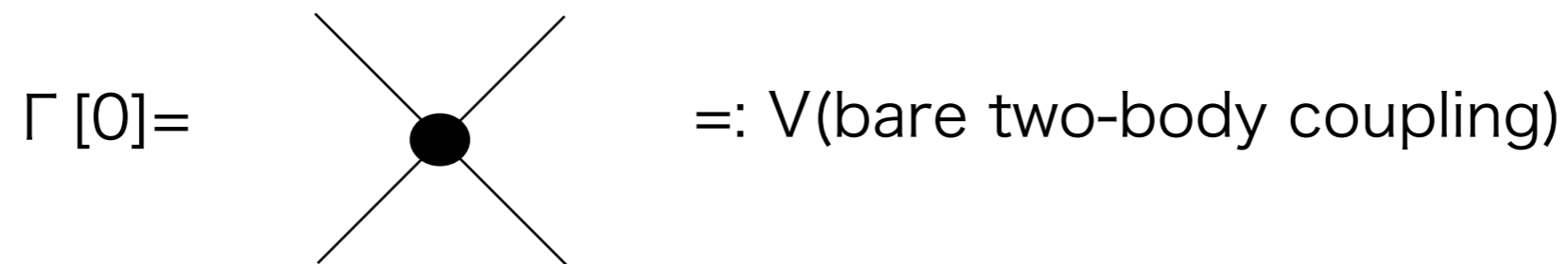
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Non-Perturbativeness of IM-SRG: Schematic

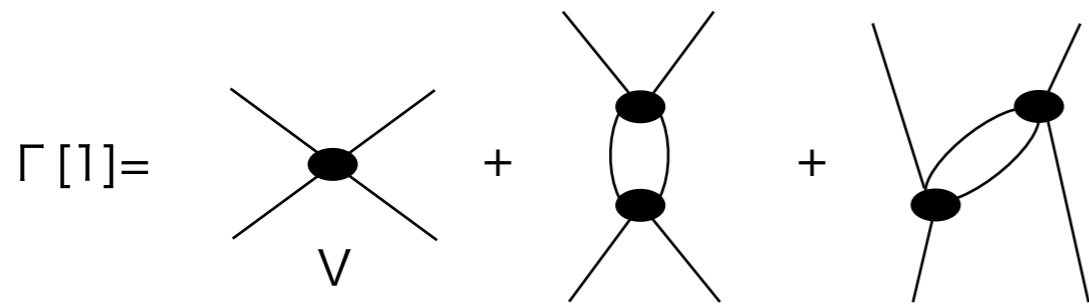
The flow equation can essentially be seen as



With the initial condition

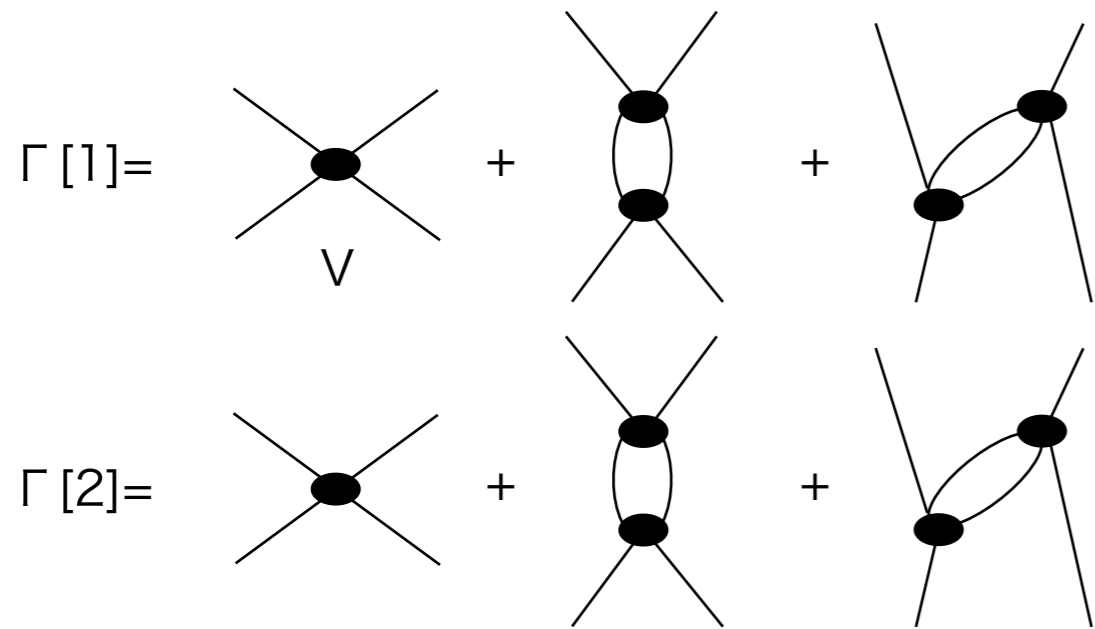


Non-Perturbativeness of IM-SRG: Schematic



Solving the flow equation step by step

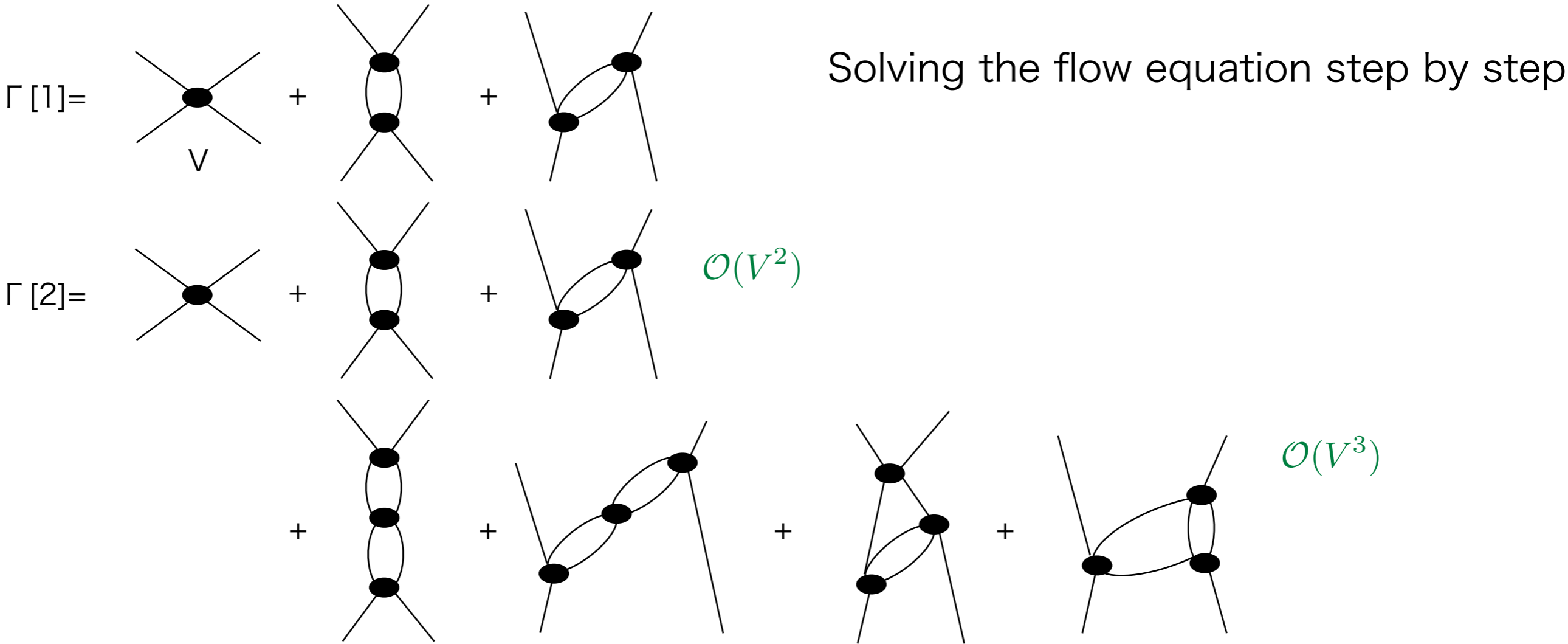
Non-Perturbativeness of IM-SRG: Schematic



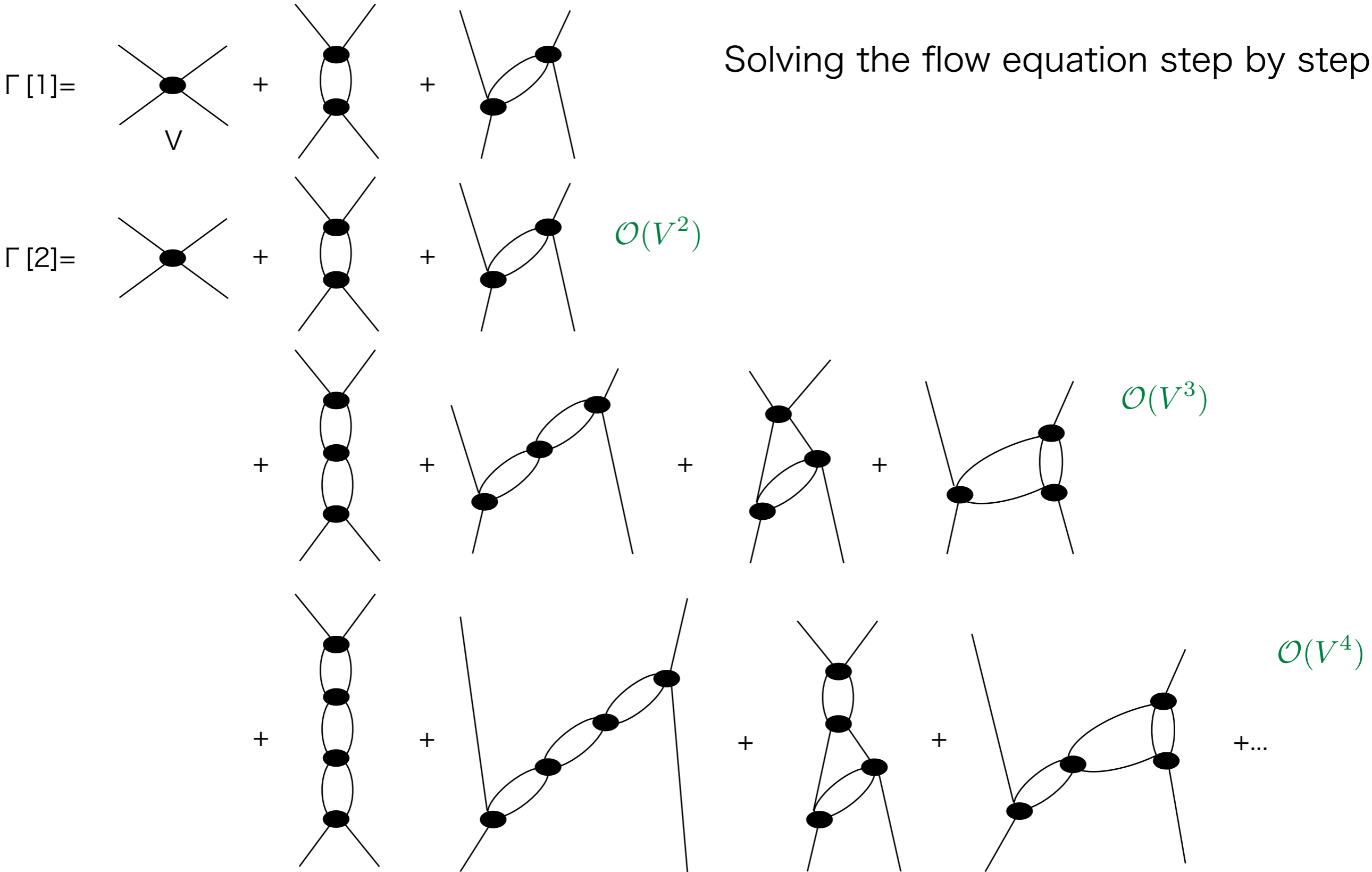
Solving the flow equation step by step

$\mathcal{O}(V^2)$

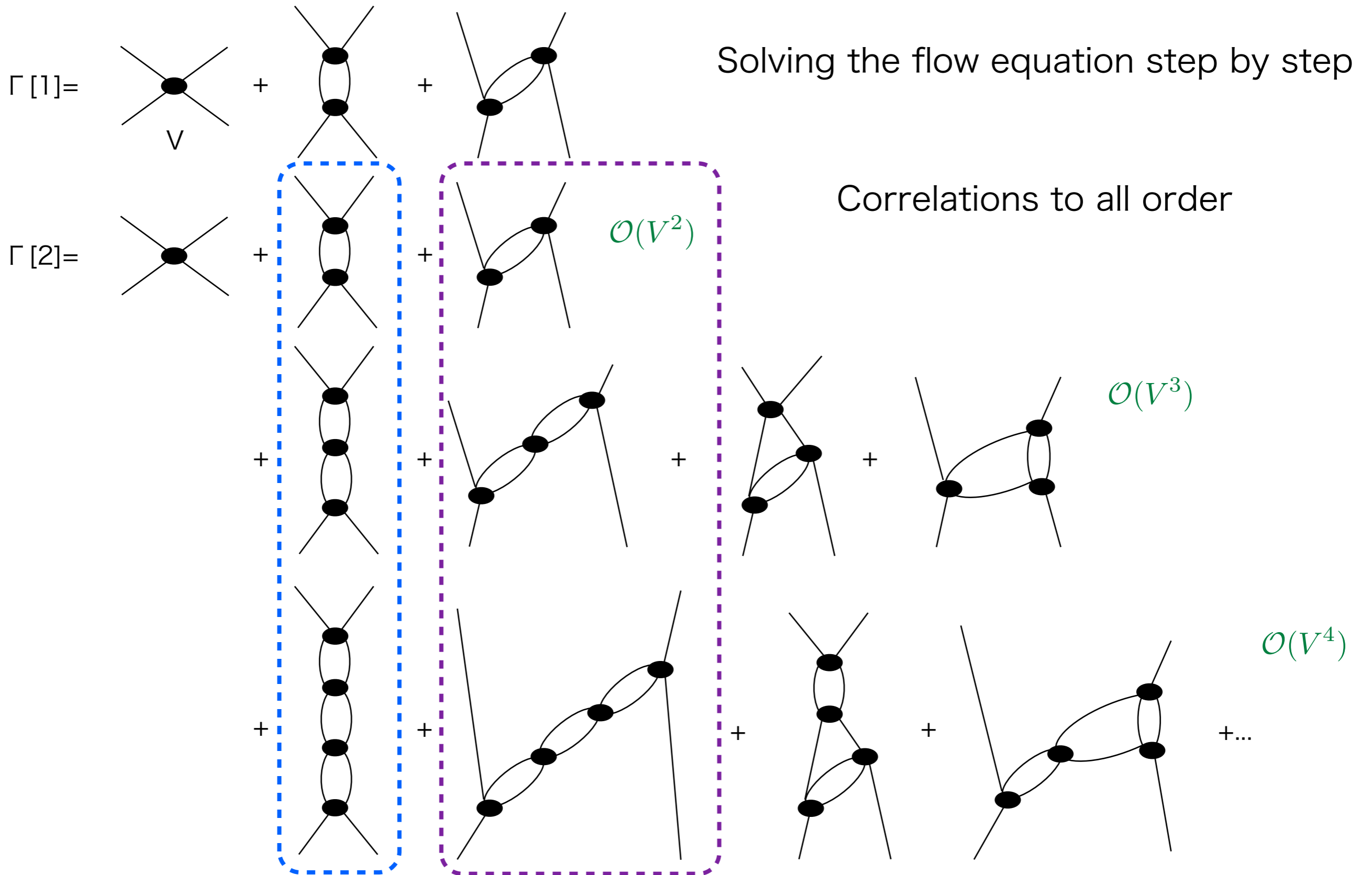
Non-Perturbativeness of IM-SRG: Schematic



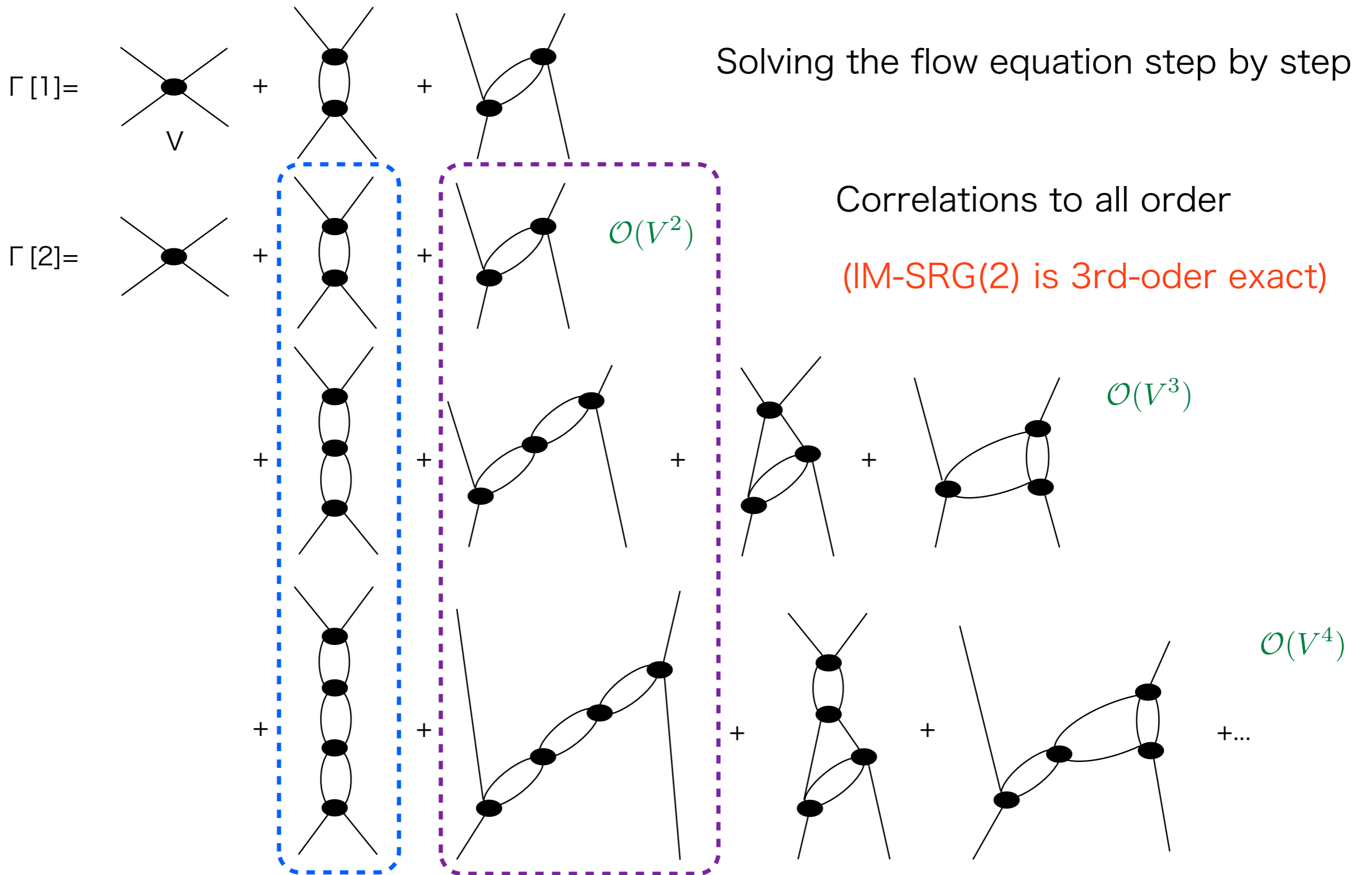
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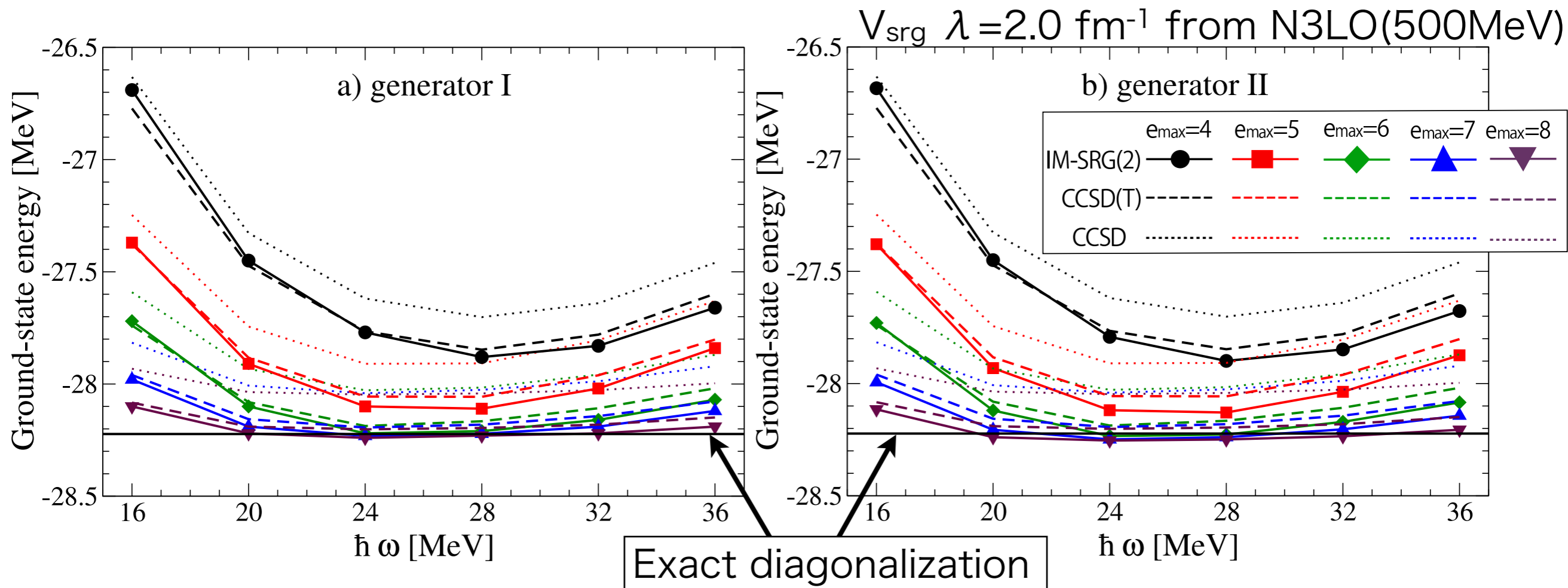
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Non-Perturbativeness of IM-SRG: Schematic



Ground-State Energy of ^4He

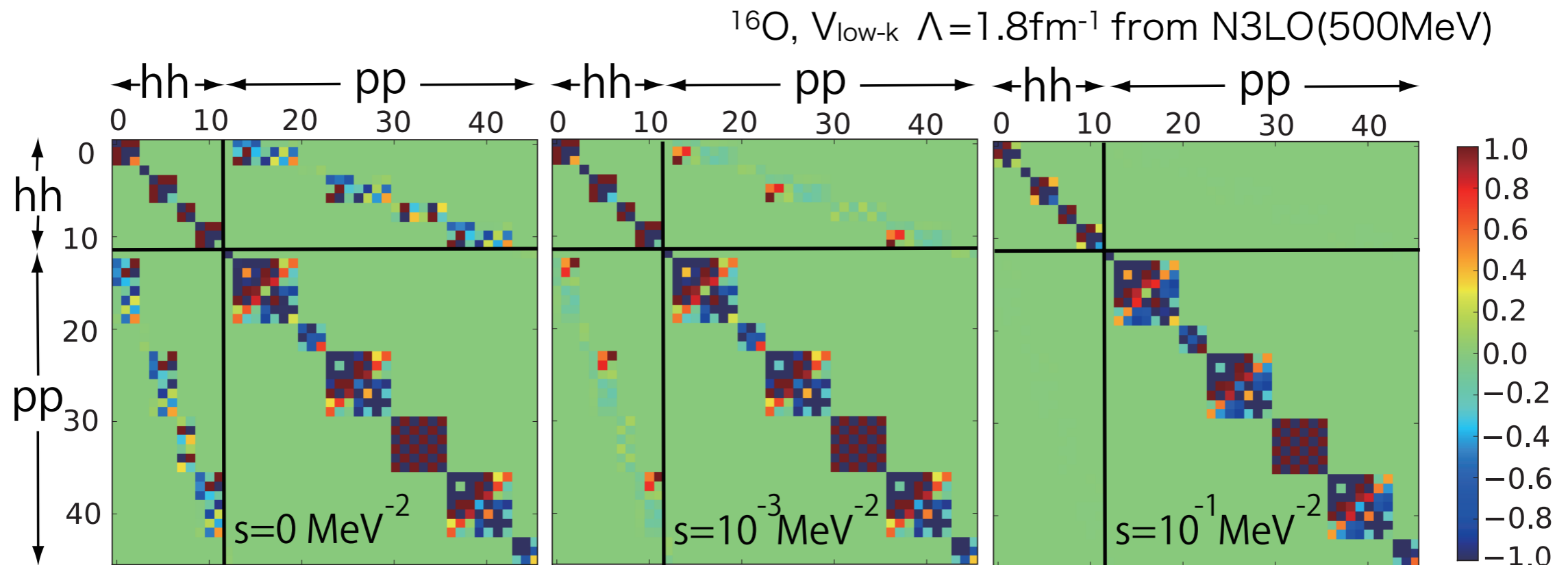


- ♣ The IM-SRG(2) for both generators are in good agreement with the CCSD(T)
- ♣ The η^I and η^{II} results agree to within 20 keV of each other.
- ♣ Essentially converged $e_{\text{max}}=8$ results falls within 20 keV of the exact NCSM.

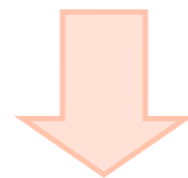
Truncation to normal-ordered two-body interaction is a controlled approximation.

Suppression of $H^{\text{od}}(s)$

η^l -evolution of the matrix elements $\Gamma^{JTz}_{abcd}(s)$ at three different steps in s .



The off-diagonal couplings in the initial Hamiltonian are rapidly driven to zero

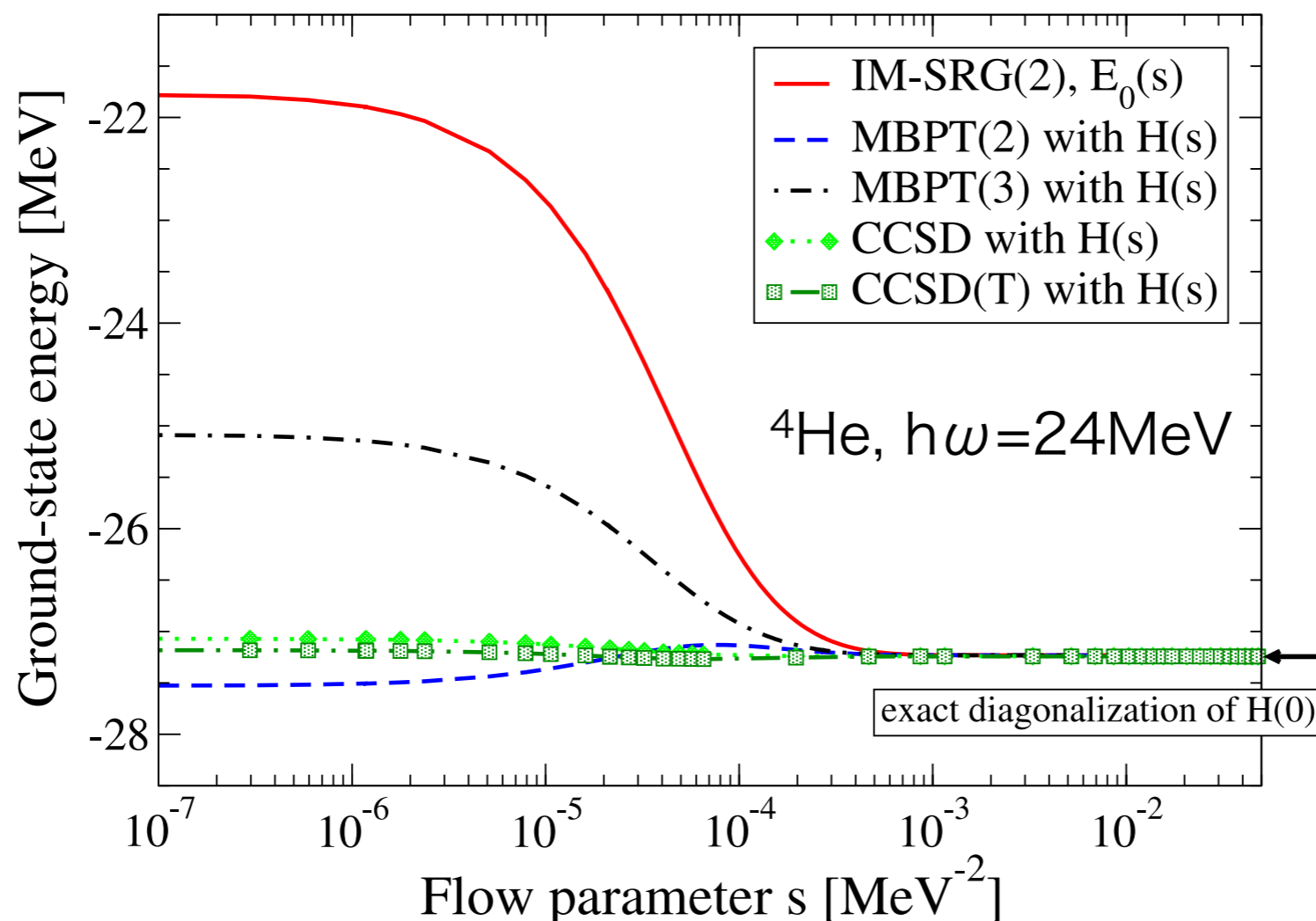


Perturbative many-body approximations become more effective in SRG evolution well before the the complete decoupling.

Non-perturbativeness

Many-body methods with the flowing Hamiltonian $H(s)$

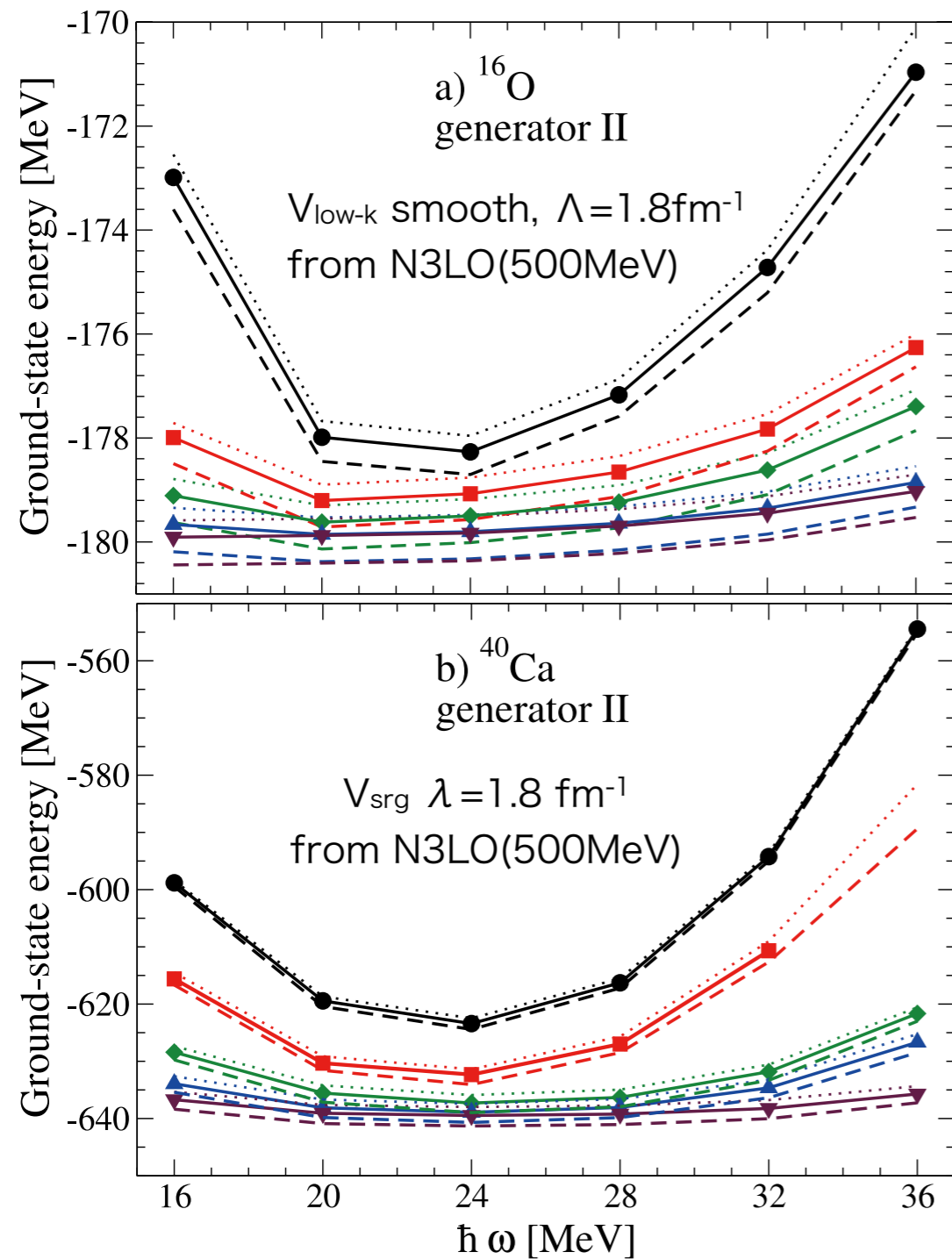
$$H(0)=T+V-T_{CM}, \quad V=V_{srg} \quad \lambda=2.0 \text{ fm}^{-1} \text{ from N3LO(500MeV)}$$



- ❖ With the initial Hamiltonian, **MBPT breaks down**.
- ❖ With increasing s , MBPT become small.
- ❖ All many-body methods approach the exact results, where the transformed Hamiltonian can be diagonalized by the simplest state.
- ❖ Almost **s -independent CCSD(T)** \implies IM-SRG(2) is controllable approximation.

The 2nd order happens to be nice
BUT the 3rd order goes bad.

Size-extensibility: Numerically manifested



- ❖ The calculations for ^{16}O , ^{40}Ca are well -converged and very good quality,
- ❖ Falling between CCSD and CCSD(T)
- ❖ IM-SRG can be used for medium-mass nuclei, probably heavier ones as well.

Summary and Outlook

Summary

- ☑ We introduced SRG evolution of Hamiltonian in many-body medium (IM-SRG).
- ☑ The flow equation is derived for finite system in M- and J-scheme representation.
- ☑ We numerically demonstrated the features of in-medium SRG
 - ☑ Decoupling of the ground state.
 - ☑ Size-extensivity
 - ☑ Non-perturbative

Summary and Outlook

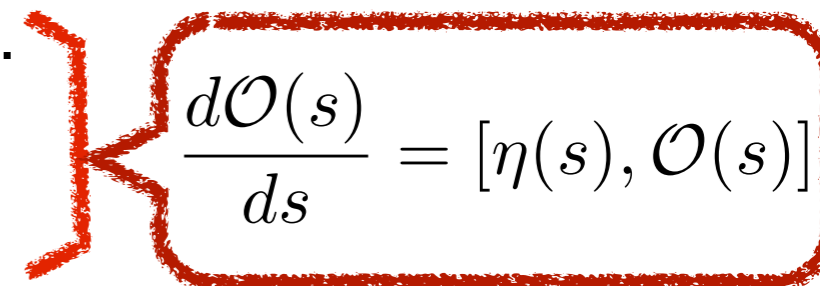
Summary

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- We numerically demonstrated the features of in-medium SRG
 - Decoupling of the ground state.
 - Size-extensivity
 - Non-perturbative

Work in Progress

- Application to heavier system ==> frontier of ab-initio method
- Derivation of **effective operator/Hamiltonian** for open-shell systems.
 - effective interaction for valence shell nucleons. <= ready for p-, sd-shell!
 - effective charge ==> B(E2) for C, Ca, Ni and Sn.
 - quenching factor for GT transition,
 - charge/matter radii
- An Initial 3NF ==> Impact of 3NF in medium, neutron-rich nuclei.

<= start with normal-ordered 3NF


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

Thanks to Collaborators

In-medium SRG

Achim Schwenk, TU Darmstadt, EMMI/GSI

Scott Bogner, NSCL/MSU

Applications to the nuclear shell-model

Taka Otsuka (Supervisor), U. Tokyo

Noritaka Shimizu, U. Tokyo

Danke schön!