Similarity Renormalization Group to the nuclear shell model

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Introduction

One of the major goals of nuclear physics

- To calculate many-body observables quantitatively starting from microscopic NN or NNN interactions.

We don't know exactly the nuclear forces.

=>To understand nucleonic interactions from more fundamental degrees of freedom.

If nucleonic interactions would be given, it is still NOT easy to calculate many-body observable.

Short-distance repulsion in nuclear forces as well as a strong tensor force.

➡ Highly non-perturbative few- and many-body system

Effective interactions for Nuclear Many-body System

Usually one overcomes this problem by

- Introducing the Brueckner G-matrix

  => Re-summation of in-medium pp scattering.

- Using RG approach, Vlowk
- Using unitary transformations
- UCOM

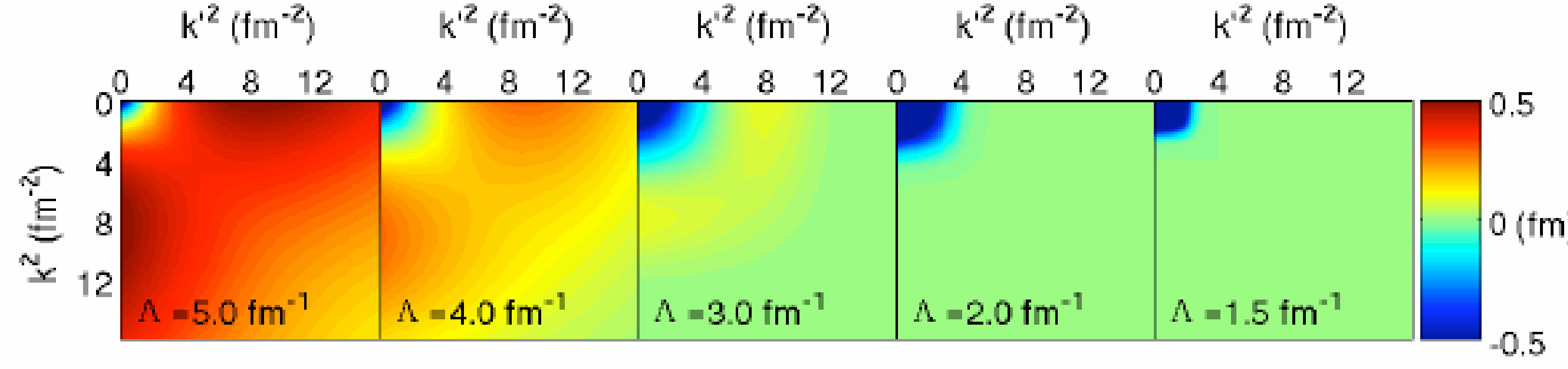
} RG equations (Using RG approach, Vlowk; Using unitary transformations)

} Unitary transformation (Using unitary transformations; UCOM)

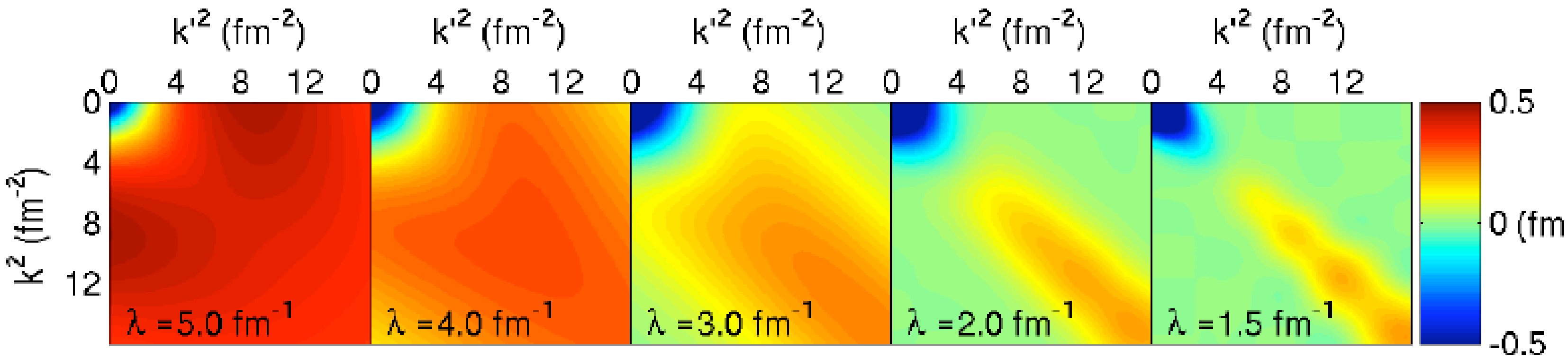
Two Types of RG transformations AV18 $^3S_1$

$$\hbar^2/M = 1$$

- $V_{low\text{-}k}$ lowers a cutoff in (k, k')



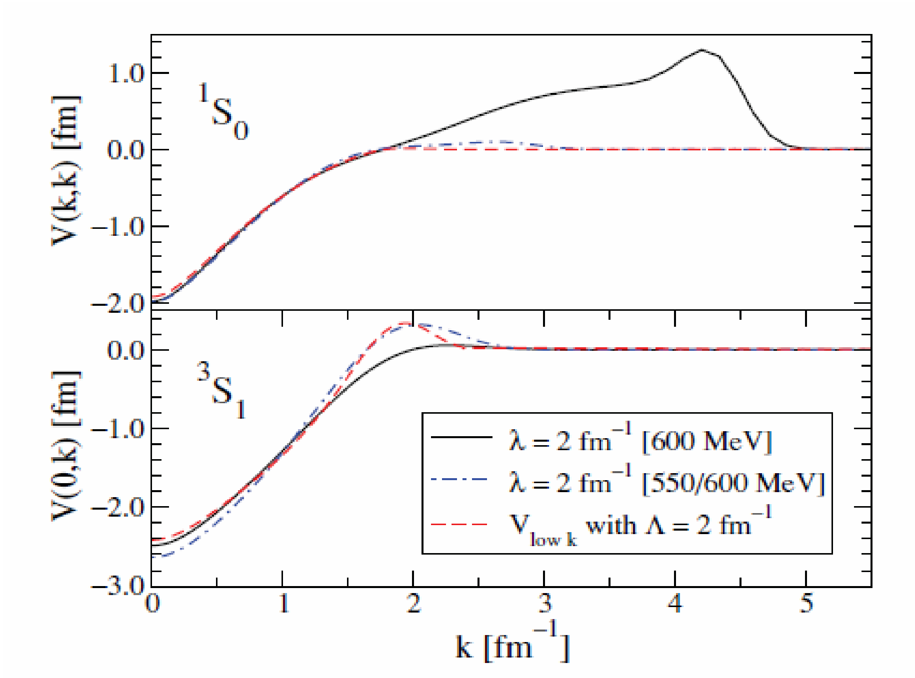
- SRG drives Hamiltonian towards the band-diagonal



Both decouple the high momentum modes, leaving **low energy NN observables unchanged**.

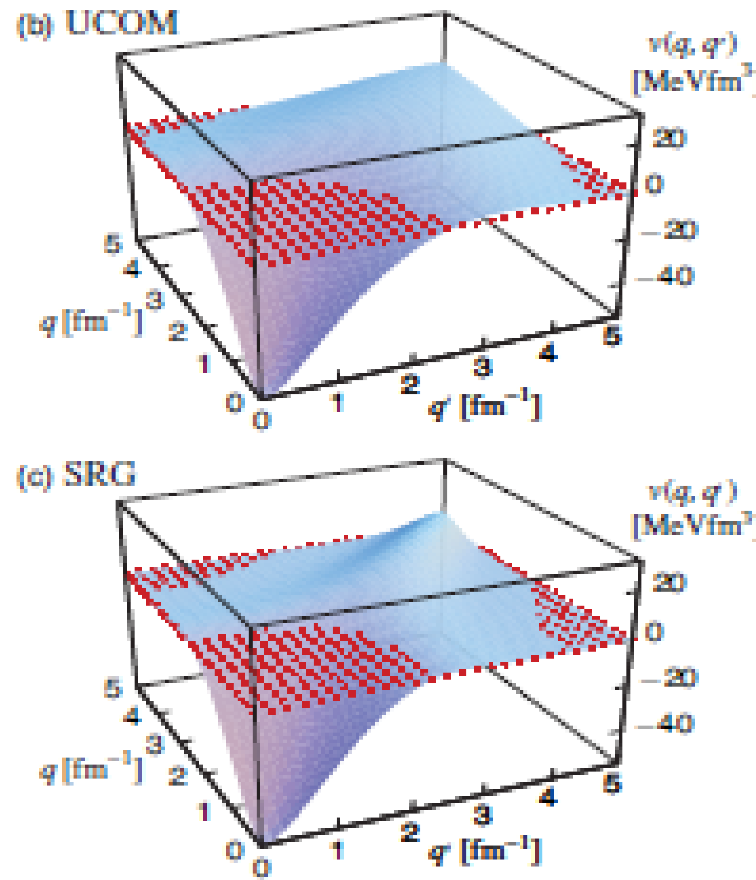
UCOM and SRG and V_{lowk}

SRG vs. V_{lowk}



S. K. Bogner, R. J. Furnstahl and R .J. Perry
PRC75, 061001(R), 2007

UCOM vs. SRG



H. Hergert and R. Roth
PRC75, 051001(R), 2007

Similarity Renormalization Group

Consider a Hamiltonian that we split into diagonal and off-diagonal parts

$$H = H_d + H_{od}$$

The SRG provides a prescription to construct the appropriate unitary transformation.

$$H(s) = U^\dagger(s) H U(s) \equiv H_d(s) + H_{od}(s),$$

$$U(0) = 1, H(0) = H$$

Taking d/ds on both sides then gives

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

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

generator of the transformation

We can formally write the unitary transformation as an s-ordered exponential,

$$U(s) = \mathcal{S} \exp\left(- \int_0^s ds' \eta(s') \right).$$

Instead of giving one unitary transformation, infinitesimal representations are given in SRG.

Wegner's Choice

The idea is to drive a Hamiltonian towards the energy diagonal $H_d|i\rangle = \epsilon_i|i\rangle$

$$\eta = [H_d, H] = [H_d, H_{od}].$$

$$\begin{cases} Tr\,(H_d H_{od}) = 0, \\ Tr\left(\frac{dH_d}{ds} H_{od}\right) = 0 \end{cases} \Rightarrow \quad \frac{d}{ds} Tr\,(H_{od}^2) = 2\,Tr(\eta^2) = -2\,Tr(\eta^\dagger \eta) \leq 0$$

$\eta^\dagger \eta$ is positive semi-definite

Design η for different things as s→∞

$$\eta(s) = [G(s), H(s)]$$

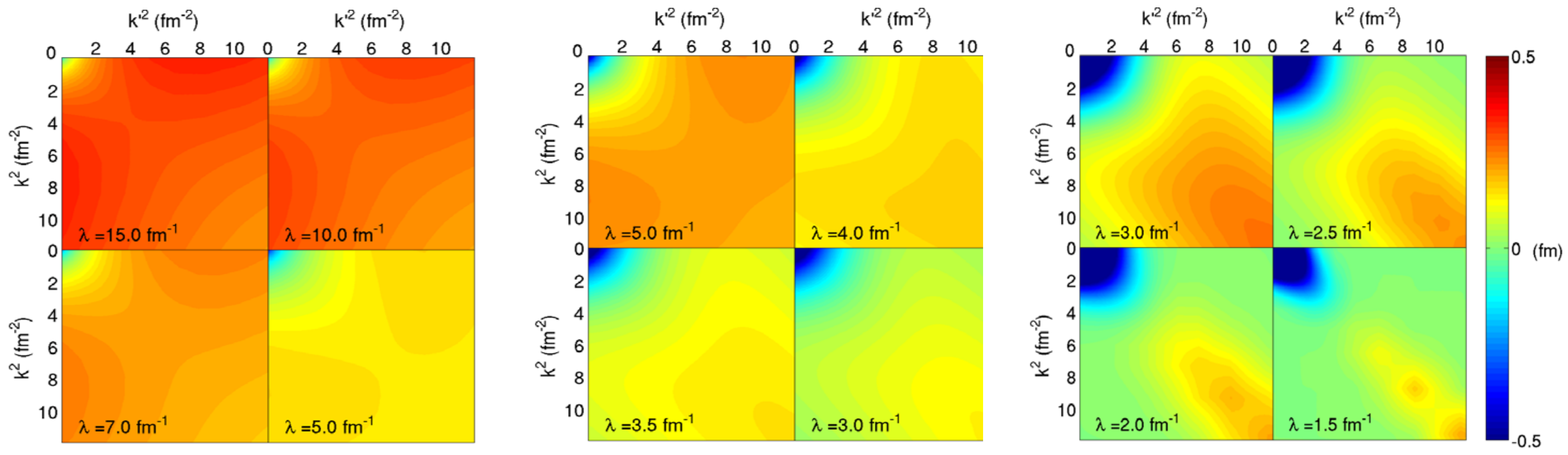
$G(s) = T$ ⇒ H(s) driven towards diagonal in k-space

$G(s) = [PH(s)P + QH(s)Q]$ ⇒ H(s) driven towards block diagonal

Free Space SRG $\eta = [T, H(s)]$

In each partial waves with $\hbar^2/M = 1$ and $\lambda = s^{-1/4}$

$$\frac{d}{ds}V_s(k,k') = -(k^2-k'^2)^2 V_s(k,k') + \frac{2}{\pi}\int_C^\infty dq q^2 (k^2+k'^2-2q^2) V_s(k,q) V_s(q,k').$$



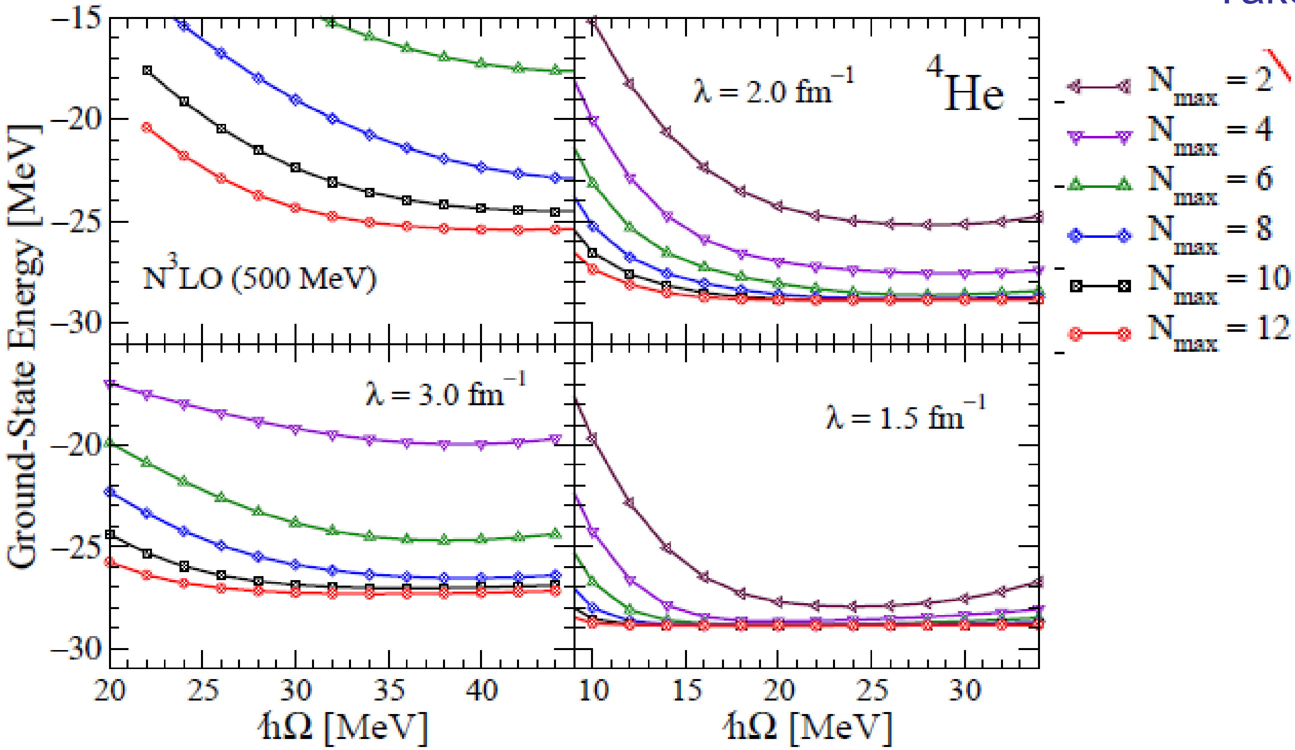
For AV18, $^3S_1$

Taken from http://www.physics.ohio-state.edu/~ntg/srg/

Free Space SRG

Full configuration interaction (FCI) calculation results

Taken by arXiv:0708.3754v2



As λ reduced (s increased) => low-k and high-k decoupled

➡ Convergence is accelerated

But λ -dependent results.

SRG and Many-body forces

SRG generates { A unitary transformed Hamiltonian
Exactly the same value for observable

→ Only if the entire Hamiltonian is kept.

NN flow is only approximately unitary

But many-body interactions are induced in the flow.

$$\frac{d}{ds}V_s = \left[\left[\sum a^\dagger a, \sum a^\dagger a^\dagger aa\right], \sum a^\dagger a^\dagger aa\right] = \cdots + \sum a^\dagger a^\dagger a^\dagger aaa + \cdots$$

In principle up to A-body term is generated.

Bare H also have this structure, for instance, $H_{EFT}=H_{1b}+H_{2b}+H_{3b}+H_{4b}+\ldots$

- For SRG to be useful for nuclear structure, the point is

Maintaining the hierarchy of many-body forces

OK if the induced terms are of natural size.

Calculate 3-body sector in the flow . (an advantage of SRG)

Normal-ordering and truncation may be sufficient.

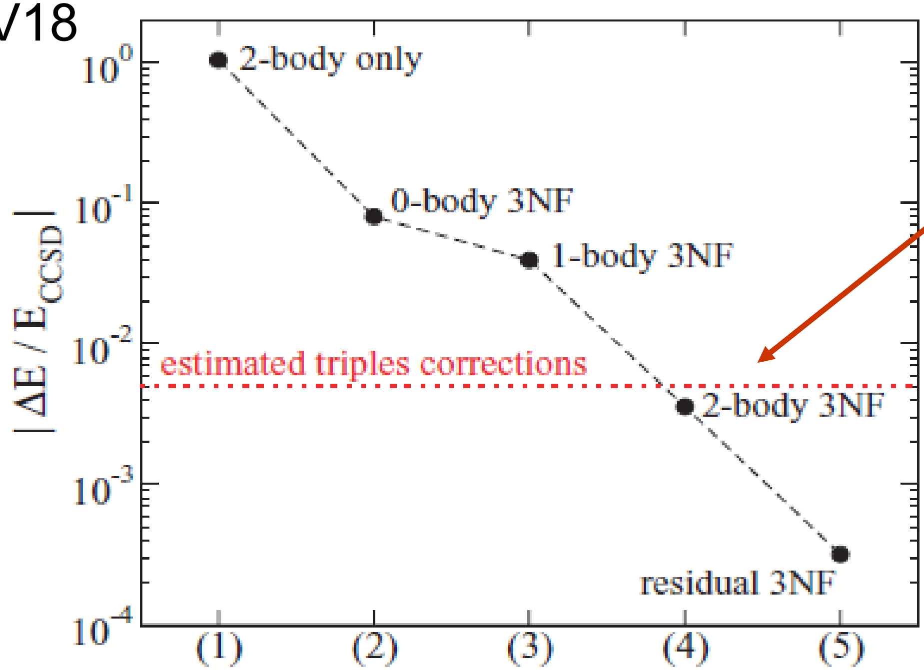
3N Interaction and Normal-Ordering

Hagen, Papenbrock, Dean, Schwenk.. PRC76, 034302 (2007)

$$H = T + V_{\mathrm{lowk}}(\Lambda) + V_{3N}(\Lambda)$$

Fitted to the data of ^{3}H and ^{4}He

from AV18



Error estimation in CCSD

Very small residual 3NF

Normal-ordering can preserve the hierarchy of Many-body forces.

In NCSM, density-dependent two-body terms are the most significant contributions of effective 3NF

Navrátil and Ormand in PRL88, 152502(2002)

In-medium SRG

Rewrite a Hamiltonian taking normal-ordering

$$\hat{H} = \sum_{ij} T_{ij} a_i^\dagger a_j + \frac{1}{2!^2} \sum_{ijkl} \langle ij|V_2|kl\rangle a_i^\dagger a_j^\dagger a_l a_k + \frac{1}{3!^2} \sum_{ijklmn} \langle ijk|V_3|lnm\rangle a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l + \cdots$$

$$= E_0 + \sum_{kk'} g_{kk'} N(k^\dagger k') + \frac{1}{2!^2} \sum_{kpqr} \Gamma_{kpqr} N(k^\dagger p^\dagger rq) + \frac{1}{3!^2} \sum_{kpqrst} \langle kpq|W|rst\rangle N(k^\dagger p^\dagger q^\dagger tsr)$$

$$E_0 = \langle H\rangle_0 = \sum_k T_{kk} n_k + \frac{1}{2} \sum_{ij} \langle ij|V_2|ij\rangle n_i n_j + \frac{1}{6} \sum_{ijk} \langle ijk|V_3|ijk\rangle n_i n_j n_k$$

$$g_{ij} = T_{ij} + \sum_k \langle ik|V_2|jk\rangle n_k + \frac{1}{2} \sum_{kl} \langle ikl|V_3|jkl\rangle n_k n_l$$

$$\langle kp|\Gamma|qr\rangle = \langle kp|V_2|qr\rangle + \frac{1}{4} \sum_i \langle kpi|V_3|qri\rangle n_i$$

3N, 4N.. forces appear as density dependence in expectation value of a core, s.p.e's and TBME's

Choose generator, following Wegner's idea

$$\hat{\eta} = [\hat{H}^d, \hat{H}^{od}] = [\hat{g}^d + \hat{\Gamma}^d, \hat{g}^{od} + \hat{\Gamma}^{od}]$$

Truncate flow equation up to Two-body normal-ordered operators

Flow equations of In-medium SRG

Generator is written as

$$\eta = \eta^{1b} + \eta^{2b}$$
$$= \sum_{k_1,k_2} \eta^{1b}_{k_1 k_2} N(a_1^\dagger a_2) + \frac{1}{4} \sum_{k_1,k_2,k_3,k_4} \eta^{2b}_{k_1 k_2 k_3 k_4} N(a_1^\dagger a_2^\dagger a_4 a_3)$$

$$\eta^{1b}_{k_1 k_2} = \sum_{k_a} \left(g^{d}_{k_1 k_a} g^{od}_{k_a k_2} - g^{od}_{k_1 k_a} g^{d}_{k_a k_2} \right)$$
$$+ \frac{1}{(2j_1+1)} \sum_J (2J+1) \left[- \sum_{k_a k_b} (n_a - n_b) g^{od}_{k_a k_b} \tilde{\Gamma}^{d,J}_{k_b k_1 k_a k_2} \right.$$
$$\left. + \frac{1}{2} \sum_{k_a k_b k_c} \left(\tilde{\Gamma}^{d,J}_{k_c k_1 k_a k_b} \tilde{\Gamma}^{od,J}_{k_a k_b k_c k_2} - \tilde{\Gamma}^{od,J}_{k_c k_1 k_a k_b} \tilde{\Gamma}^{d,J}_{k_a k_b k_c k_2} \right) (\bar{n}_a \bar{n}_b n_c + n_a n_b \bar{n}_c) \right]$$

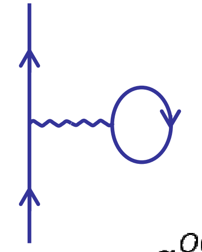
Flow equations of In-medium SRG

$$
\begin{aligned}
\tilde{\eta}^{2b,J}_{k_1k_2k_3k_4} &= \sum_{k_a}\left(g^{d}_{k_1k_a}\tilde{\Gamma}^{od,J}_{k_ak_2k_3k_4} + g^{d}_{k_2k_a}\tilde{\Gamma}^{od,J}_{k_1k_ak_3k_4} - g^{d,1b}_{k_ak_3}\tilde{\Gamma}^{od,J}_{k_1k_2k_ak_4} - g^{d}_{k_ak_4}\tilde{\Gamma}^{od,J}_{k_1k_2k_3k_a}\right) \\
&- \sum_{k_a}\left(g^{od}_{k_1k_a}\tilde{\Gamma}^{d,J}_{k_ak_2k_3k_4} + g^{od}_{k_2k_a}\tilde{\Gamma}^{d,J}_{k_1k_ak_3k_4} - g^{od}_{k_ak_3}\tilde{\Gamma}^{d,J}_{k_1k_2k_ak_4} - g^{od}_{k_ak_4}\tilde{\Gamma}^{d,J}_{k_1k_2k_3k_a}\right) \\
&+ \frac{1}{2}\sum_{k_ak_b}(1-n_a-n_b)\left(\tilde{\Gamma}^{d,J}_{k_1k_2k_ak_b}\tilde{\Gamma}^{od,J}_{k_ak_bk_3k_4} - \tilde{\Gamma}^{od,J}_{k_1k_2k_ak_b}\tilde{\Gamma}^{d,J}_{k_ak_bk_3k_4}\right) \\
&- \sum_{k_ak_b}(n_a-n_b)\sum_{J_1J_2}(2J_1+1)(2J_2+1)(-1)^{j_1+j_3+J_1-J_2} \\
&\times \left[(-1)^J\begin{Bmatrix} j_a & j_4 & J_1 \\ j_1 & J & j_2 \\ J_2 & j_3 & j_b \end{Bmatrix}\left(\tilde{\Gamma}^{d,J_1}_{k_bk_2k_ak_4}\tilde{\Gamma}^{od,J_2}_{k_ak_1k_bk_3} - \tilde{\Gamma}^{od,J_1}_{k_bk_2k_ak_4}\tilde{\Gamma}^{d,J_2}_{k_ak_1k_bk_3}\right)\right. \\
&\left. - \begin{Bmatrix} j_a & j_4 & J_1 \\ j_2 & J & j_1 \\ J_2 & j_3 & j_b \end{Bmatrix}\left(\tilde{\Gamma}^{d,J_2}_{k_ak_2k_bk_3}\tilde{\Gamma}^{od,J_1}_{k_bk_1k_ak_4} - \tilde{\Gamma}^{od,J_2}_{k_ak_2k_bk_3}\tilde{\Gamma}^{d,J_1}_{k_bk_1k_ak_4}\right)\right]
\end{aligned}
$$

Flow equations of In-medium SRG

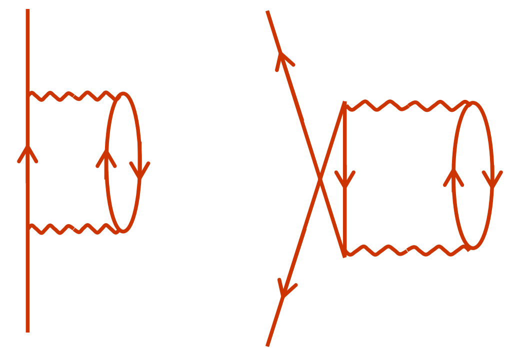
$$\frac{d}{ds}E_0 = \frac{1}{2}\sum_{k_1k_2k_3k_4}\sum_J (2J+1)\tilde{\eta}^{2b,J}_{k_1k_2k_3k_4}\tilde{\Gamma}^{2b,J}_{k_1k_2k_3k_4} n_1 n_2 \bar{n}_3 \bar{n}_4 + \sum_{k_1k_2}(2j_1+1)\eta^{1b}_{k_1k_2} g^{od}_{k_1k_2}(n_1 - n_2)$$

$$\frac{d}{ds}g_{k_1k_2} = \sum_{k_a}\left(\eta^{1b}_{k_1k_a} g_{k_ak_2} - g_{k_1k_a}\eta^{1b}_{k_ak_2}\right)$$



$$+\frac{1}{(2j_1+1)}\sum_J (2J+1)\left[\sum_{k_ak_b}(n_a - n_b)\left\{\eta^{1b}_{k_ak_b}\tilde{\Gamma}^J_{k_bk_1k_ak_2} - g^{od}_{k_ak_b}\tilde{\eta}^{2b,J}_{k_bk_1k_ak_2}\right\}\right.$$

$$\left.\frac{1}{2}\sum_{k_ak_bk_c}\left(\tilde{\eta}^{2b,J}_{k_ck_1k_ak_b}\tilde{\Gamma}^J_{k_ak_bk_ck_2} - \tilde{\Gamma}^J_{k_ck_1k_ak_b}\tilde{\eta}^{2b,J}_{k_ak_bk_ck_2}\right)(\bar{n}_a\bar{n}_b n_c + n_a n_b \bar{n}_c)\right]$$



Flow equations of In-medium SRG

$$\frac{d}{ds}\tilde{\Gamma}^{J}_{k_1 k_2 k_3 k_4} = \sum_{k_a}\left(\eta^{1b}_{k_1 k_a}\tilde{\Gamma}^{J}_{k_a k_2 k_3 k_4} + \eta^{1b}_{k_2 k_a}\tilde{\Gamma}^{J}_{k_1 k_a k_3 k_4} - \eta^{1b}_{k_a k_3}\tilde{\Gamma}^{J}_{k_1 k_2 k_a k_4} - \eta^{1b}_{k_a k_4}\tilde{\Gamma}^{J}_{k_1 k_2 k_3 k_a}\right)$$

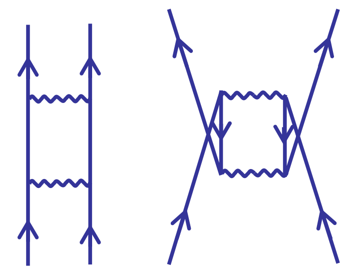
$$- \sum_{k_a}\left(g_{k_1 k_a}\tilde{\eta}^{2b,J}_{k_a k_2 k_3 k_4} + g_{k_2 k_a}\tilde{\eta}^{2b,J}_{k_1 k_a k_3 k_4} - g_{k_a k_3}\tilde{\eta}^{2b,J}_{k_1 k_2 k_a k_4} - g_{k_a k_4}\tilde{\eta}^{2b,J}_{k_1 k_2 k_3 k_a}\right)$$

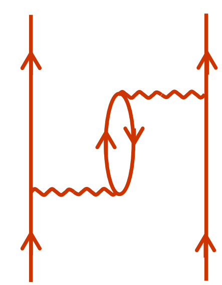
$$+ \frac{1}{2}\sum_{k_a k_b}(1 - n_a - n_b)\left(\tilde{\eta}^{2b,J}_{k_1 k_2 k_a k_b}\tilde{\Gamma}^{J}_{k_a k_b k_3 k_4} - \tilde{\Gamma}^{J}_{k_1 k_2 k_a k_b}\tilde{\eta}^{2b,J}_{k_a k_b k_3 k_4}\right)$$

$$- \sum_{k_a k_b}(n_a - n_b)\sum_{J_1 J_2}(2J_1 + 1)(2J_2 + 1)(-1)^{j_1 + j_3 + J_1 - J_2}$$

$$\times\left[(-1)^{J}\begin{Bmatrix} j_a & j_4 & J_1 \\ j_1 & J & j_2 \\ J_2 & j_3 & j_b \end{Bmatrix}\left(\tilde{\eta}^{2b,J_1}_{k_b k_2 k_a k_4}\tilde{\Gamma}^{J_2}_{k_a k_1 k_b k_3} - \tilde{\Gamma}^{J_1}_{k_b k_2 k_a k_4}\tilde{\eta}^{2b,J_2}_{k_a k_1 k_b k_3}\right)\right.$$

$$\left. - \begin{Bmatrix} j_a & j_4 & J_1 \\ j_2 & J & j_1 \\ J_2 & j_3 & j_b \end{Bmatrix}\left(\tilde{\eta}^{2b,J_2}_{k_a k_2 k_b k_3}\tilde{\Gamma}^{J_1}_{k_b k_1 k_a k_4} - \tilde{\Gamma}^{J_2}_{k_a k_2 k_b k_3}\tilde{\eta}^{2b,J_1}_{k_b k_1 k_a k_4}\right)\right]$$





Perturbative content of SRG

Example: homogeneous system like NM

In momentum basis, g is diagonal ➔ Flow eqs. can be simplified

$$g_{ab} = \delta_{ab} g_{aa} = \delta_{ab} f_a$$

The flow equations at leading order are

$$\eta^{2b,J}_{k_1 k_2 k_3 k_4} = (f_1 + f_2 - f_3 - f_4) \tilde{\Gamma}^{J}_{k_1 k_2 k_3 k_4}$$

$$\begin{cases} \frac{d}{ds} E_0(s) = \frac{1}{2} \sum_J (2J+1) \sum_{k_1 k_2 k_3 k_4} \tilde{\eta}^{2b,J}_{k_1 k_2 k_3 k_4} \tilde{\Gamma}^{2b,J}_{k_1 k_2 k_3 k_4} n_1 n_2 \bar{n}_3 \bar{n}_4 \\ \frac{d}{ds} f_a(s) = 0 \\ \frac{d}{ds} \tilde{\Gamma}^{J}_{k_1 k_2 k_3 k_4} = -(f_1 + f_2 - f_3 - f_4)^2 \tilde{\Gamma}^{od,J}_{k_1 k_2 k_3 k_4} \end{cases}$$

Solution for E_0 up to 2nd order in the bare coupling.

$$E_0(s) = E_0(0) + \underline{\frac{1}{2} \sum_J (2J+1) \sum_{k_1 k_2 k_3 k_4} \frac{|\tilde{\Gamma}^{od,J}_{k_1 k_2 k_3 k_4}|^2}{f_1 + f_2 - f_3 - f_4} \left(1 - e^{-(f_1+f_2-f_3-f_4)^2 s}\right) n_1 n_2 \bar{n}_3 \bar{n}_4}$$

Correlation energy

As s increases, correlation energy is shuffled into non-interacting VEV (HF).

Preliminary calculations

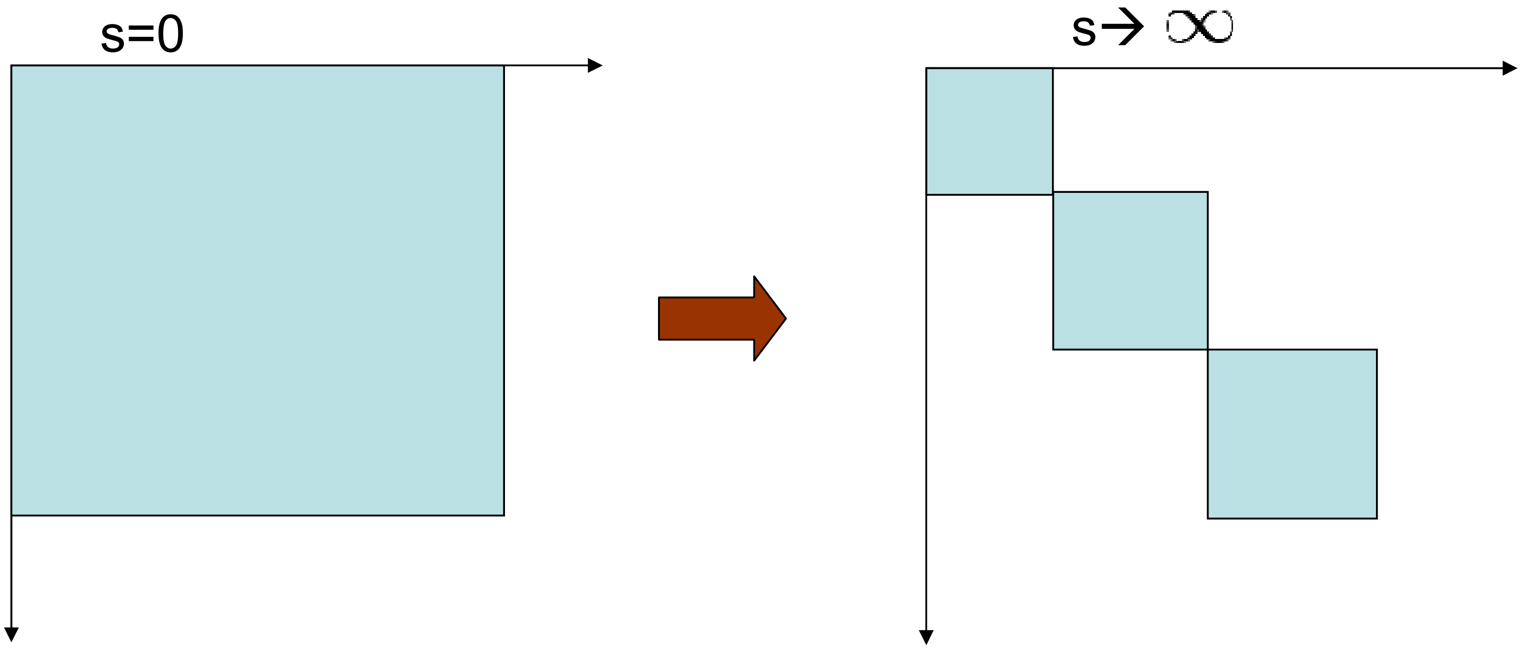
Wegner's choice for the generator

$$\hat{\eta} = [\hat{H}^d, \hat{H}^{od}] = [\hat{g}^d + \hat{\Gamma}^d, \hat{g}^{od} + \hat{\Gamma}^{od}]$$

$$\Gamma^d_{1234} = 0 \quad (\epsilon_1 + \epsilon_2 \neq \epsilon_3 + \epsilon_4), \qquad \Gamma^{od}_{1234} = 0 \quad (\epsilon_1 + \epsilon_2 = \epsilon_3 + \epsilon_4),$$

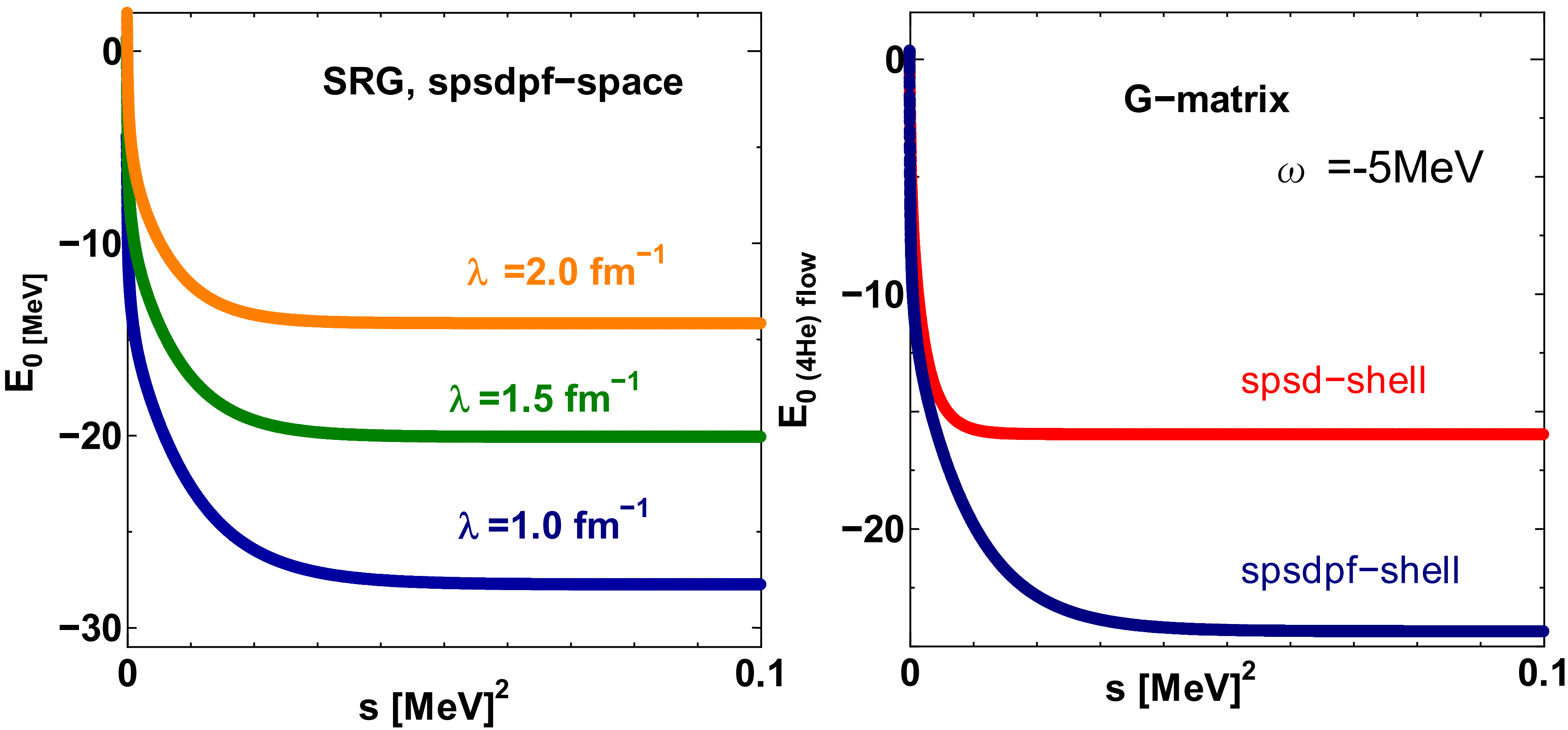
$$g^d_{12} = 0 \quad (\epsilon_1 \neq \epsilon_2), \qquad g^{od}_{12} = 0 \quad (\epsilon_1 = \epsilon_2).$$

$$\epsilon_a = \epsilon_{n_a l_a j_a} = \hbar\omega(2n_a + l_a + 3/2)$$



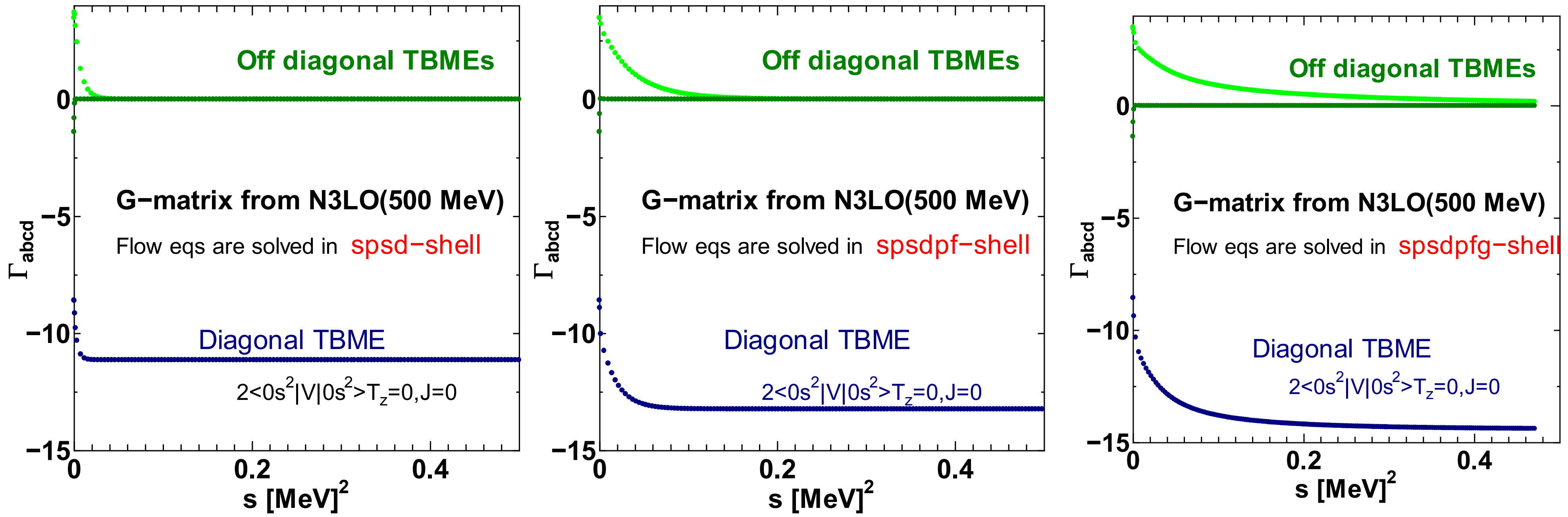
E_0 (^{4}He) flow (solved in small spaces) [N3LO(500MeV)]

V_{NN} → G-matrix / Free space SRG } = as an input of In-medium SRG



We need lager space to make the flow more reliable.

Observation



Energy off-diagonal matrix elements vanish after the flow.

$$\Gamma_{1234} \to 0 \quad \text{if} \;\; \epsilon_1 + \epsilon_2 \neq \epsilon_3 + \epsilon_4$$

Observations

We don't have to solve cluster problems.

Energy off-diagonal matrix elements vanish after the flow.

$$\Gamma_{1234} \rightarrow 0 \quad \text{if} \;\; \epsilon_1 + \epsilon_2 \neq \epsilon_3 + \epsilon_4$$

There are some cross-shell TBME's after the flow

$$\langle 0s1p|V|0s1p\rangle \;\; \langle 0s1s|V|0s1s\rangle \;\; \langle 0s0dV|0s0d\rangle \cdots$$

Initial value-dependent (due to the small space flow?)

Summary

- We have derived the flow equations for In-medium SRG in M- and J-scheme basis.
- Non-perturbative path to the nuclear shell model.
- Current choice of the generator can get stable flow.
- Enegy off-diagonal M.E's are well suppressed after the flow.
- HF covers the dominant part of the correlation energy ➔ Shell Model
- There are some cross-shell TBME's after the flow ➔ physical meaning

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- We need large space flow to see the convergence.

  ➔direct connection between bare nuclear forces and the nuclear shell model.
- 3NF in the initial Hamiltonian
- 3NF in the normal-ordered Hamiltonian ➔ the magnitude of the induced 3NF
- In-medium SRG for effective operator O_{eff} as well as H_{eff}.

Collaborators

- Achim Schwenk (TRIUMF)
- Scott Bogner (MSU)
- Takaharu Otsuka (Tokyo)