Operator evolution from the SRG and the Magnus expansion

Journal club, Chenrong Ding

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Abstract & Introduction

The Magnus expansion is an efficient alternative to solving similarity renormalization group (SRG) flow equations with high-order, memory-intensive ordinary differential equation solvers. The numerical simplifications it offers for operator evolution are particularly valuable for in-medium SRG calculations, though challenges remain for difficult problems involving intruder states. Here we test the Magnus approach in an analogous but more accessible situation, which is the free-space SRG treatment of the spurious bound states arising from a leading-order chiral effective field theory (EFT) potential with very high cutoffs. We show that the Magnus expansion passes these tests and then use the investigations as a springboard to address various aspects of operator evolution that have renewed relevance in the context of the scale and scheme dependence of nuclear processes. These aspects include SRG operator flow with band- versus block-diagonal generators, universality for chiral EFT Hamiltonians and associated operators with different regularization schemes, and the impact of factorization arising from scale separation. Implications for short-range correlations physics and the possibilities for reconciling high- and low-resolution treatments of nuclear structure and reactions are discussed.

- The free-space SRG
- Band- and block-diagonal generators
- The Magnus expansion
- Universality of chiral EFT Hamiltonians and associated operators

Abstract & Introduction

- **The free-space SRG**

$$H = T_{rel}(k,k') + V(k,k')$$

- H is represented in the relative-momentum space
- $V(k,k')$ from the chiral NN interaction

The SRG decouples **low-** and **high-momentum** scales in the Hamiltonian by applying a continuous unitary transformation $U(s)$

$$H(s) = U(s)H(0)U^{\dagger}(s),$$

where H could be replaced by any other operator O. One can find the above equation by solving a differential flow equation

$$\frac{dH(s)}{ds} = [\eta(s), H(s)], \text{where } \eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s).$$

For the free-space SRG, the generator is typically defined as a commutator $\eta(s) = [G, H(s)]$, where G specifies the type of flow.

Abstract & Introduction

- **Band- and block-diagonal generators**

By setting $G = H_D(s)$ (Wegner generator) or $G = T_{rel}$, the diagonal of the Hamiltonian, the Hamiltonian is driven to **band-diagonal** form. For band-diagonal decoupling, it is convenient to define $\lambda = s^{-1/4}$, which roughly measures **the width of the band-diagonal** in the decoupled Hamiltonian.

For **block-diagonal** decoupling, G is formed by splitting the Hamiltonian into low- and high-momentum subblocks as specified by a **momentum separation scale** Λ_{BD}

$$G = \begin{bmatrix} PH(s)P & 0 \\ 0 & QH(s)Q \end{bmatrix} = H_{BD}(s).$$

Here $P = \theta(\Lambda_{BD} - k)$ and $Q = \theta(k - \Lambda_{BD})$ are low- and high- momentum projection operators. In this case, Complete decoupling of the blocks is in principle only reached in the $s \to \infty$ limit.

The Magnus expansion

The Magnus expansion is a method for solving an initial value problem associated with a **linear ordinary differential equation**. With the definition $U(s) = e^{\Omega(s)}$, one have

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

$$\frac{d\Omega(s)}{ds} = U^{\dagger}(s)\eta(s)U(s) = e^{-\Omega(s)}\eta(s)e^{\Omega(s)} = \eta(s) - [\Omega(s), \eta(s)] + \cdots$$

$\Omega(s)$ is expanded as a power series in $\eta(s)$

$$\Omega(s) = \sum_{n=1}^{\infty} \Omega_n(s), \qquad \begin{cases} \Omega_1(s) = \int_0^s ds_1 \eta(s_1), \\ \Omega_2(s) = \frac{1}{2}\int_0^s ds_1 \int_0^{s_1} ds_2 [\eta(s_1), \eta(s_2)], \\ \Omega_3(s) = \cdots \end{cases}$$

Thus the derivative of $\Omega(s)$ is $\frac{d\Omega(s)}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega}^{k}(\eta)$, where B_k is the Bernoulli numbers,$ad_{\Omega}^{0}(\eta) = \eta(s)$ and $ad_{\Omega}^{k}(\eta) = \left[\Omega(s), ad_{\Omega}^{k-1}(\eta)\right]$.

Abstract & Introduction

➢ The Magnus expansion

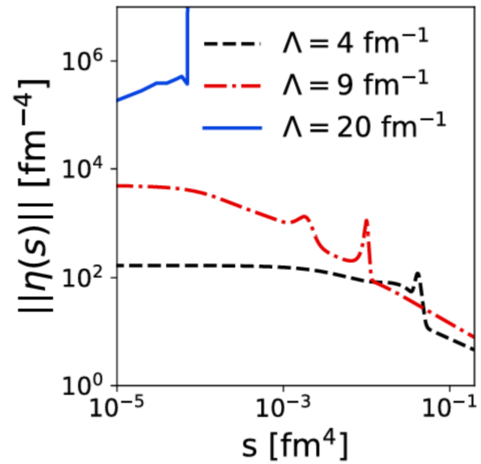
Under the Magnus form of flow equation, the evolved operator can be evaluated by

$$O(s) = e^{\Omega(s)} O(0) e^{-\Omega(s)} = \sum_{k=0}^{\infty} \frac{1}{k!} ad_{\Omega}^{k}(O(0)) .$$

Comparing to the conventional form $\frac{dO(s)}{ds} = [\eta(s), O(s)]$, the Magnus form would be much **more convenient to evolve several operators at a time**.

One of motivations of this work!

* **Convergence issue in the Magnus expansion**: when $\eta(s)$ grows as s increases, $\Omega(s)$ will grows large. The **convergence is satisfied** if $\int_0^S ||\eta(s)||ds < \pi$, where $||\eta(s)|| = \sqrt{\sum_{ij} \eta(s)_{ij}^2}$ is **the Frobenius norm**.



$s \approx 10^{-4}\mathrm{fm}^4$
$\lambda \approx 10\mathrm{fm}^{-1}$

LO potentials in the $^3S_1 - {}^3D_1$ coupled channel, $G = H_D$

Abstract & Introduction

➢ **Universality of chiral EFT Hamiltonians and associated operators**

- While interactions from chiral EFT have become the standard choice for ab initio calculations of nuclei, they are **not unique**, even when restricted to the commonly used Weinberg power counting, because of **many choices for regularization schemes and fitting protocols and even degrees of freedom** (i.e., with or without Δ).

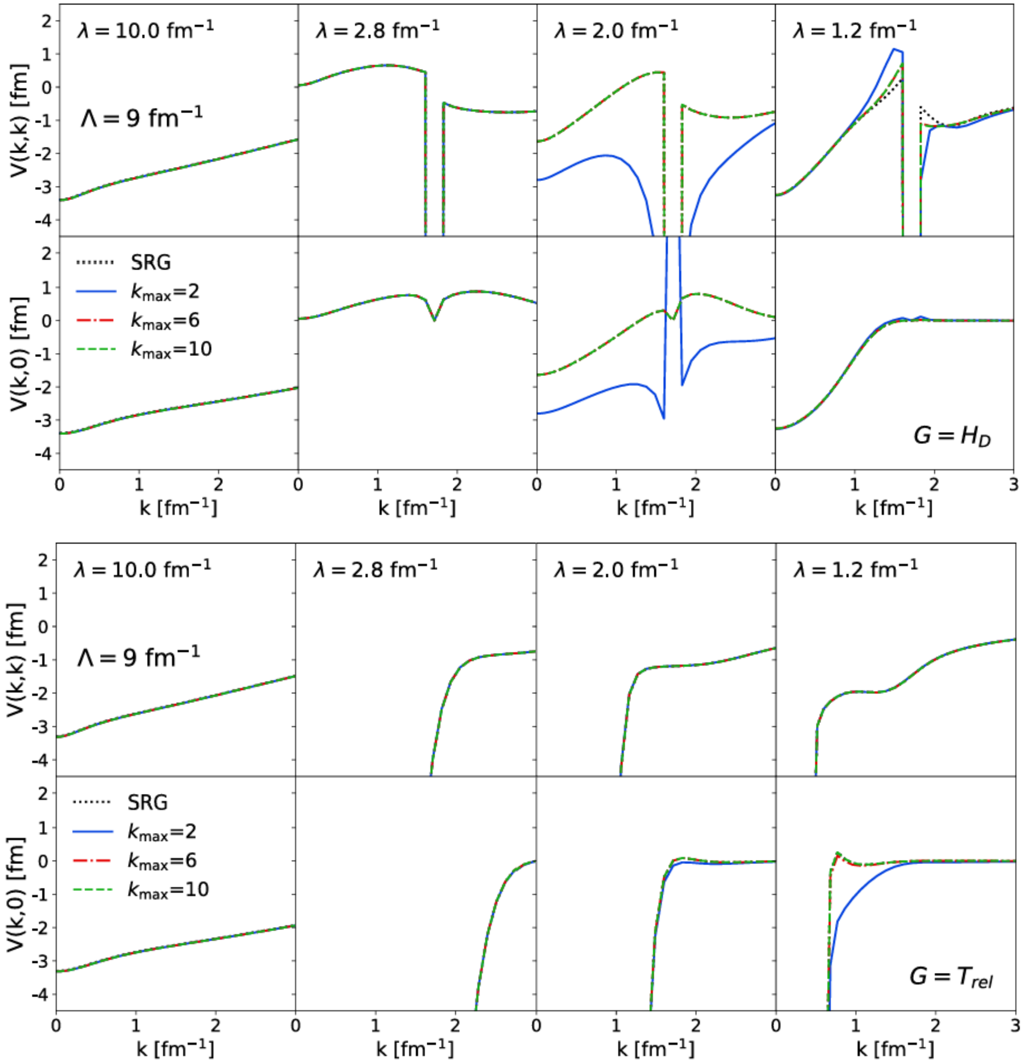
- By virtue of fitting to the same data or phase shifts, different chiral EFT potentials generate close to the same S matrix in the energy range where there is a good fit; However, **matrix elements of the potentials in momentum space** differ significantly based on **the EFT order and the choice of regulator function and cutoff (scale and scheme dependence).**

Universality: the momentum-space matrix elements based on different EFT order, regulator function and cutoff tend to be similar with the SRG-evolution.

Whether the universality holds for modern chiral potentials but also the other operators.

Another motivations of this work!

- **The k-convergence of Magnus expansion**



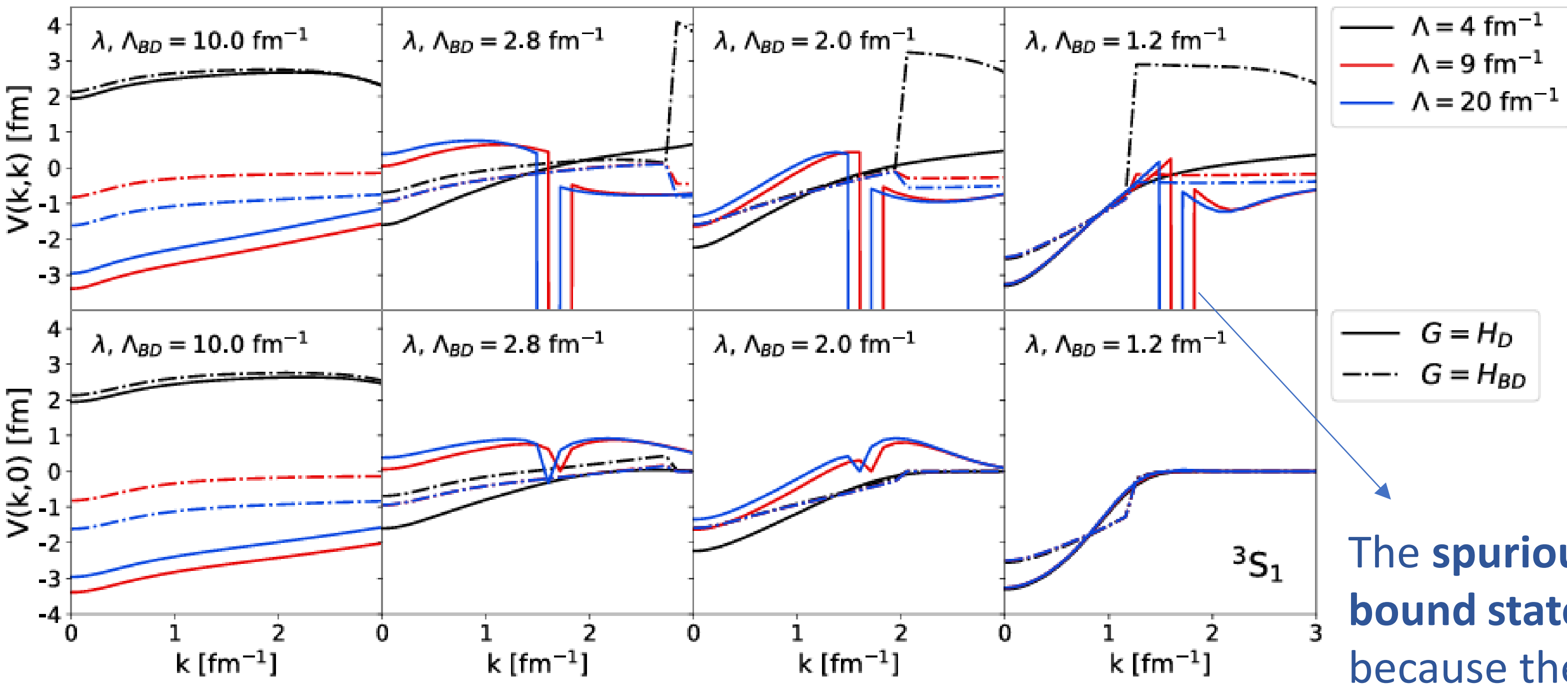
$$\frac{d\Omega(s)}{ds} = \sum_{k=0}^{k_{max}} \frac{B_k}{k!} ad_{\Omega}^{k}(\eta)$$

Taking higher values of k_{max}, the Magnus evolution approaches the SRG evolution.

- **Universality of LO potentials with different cutoffs**

* (non-local) regulator: $V_\Lambda(q',q) = R(q')V(q',q)R(q)$, with $R(q) = \exp(-(q^{2n}/\Lambda^{2n}))$, where Λ is cutoff.

With Wegner (solid) and block-diagonal (dashed) generators:



* For H_{BD} generators, λ is fixed at $1.2\ \mathrm{fm}^{-1}$.

The **spurious, deeply bound states** arise because the potentials are not renormalizable, thus it is regulator-dependent.

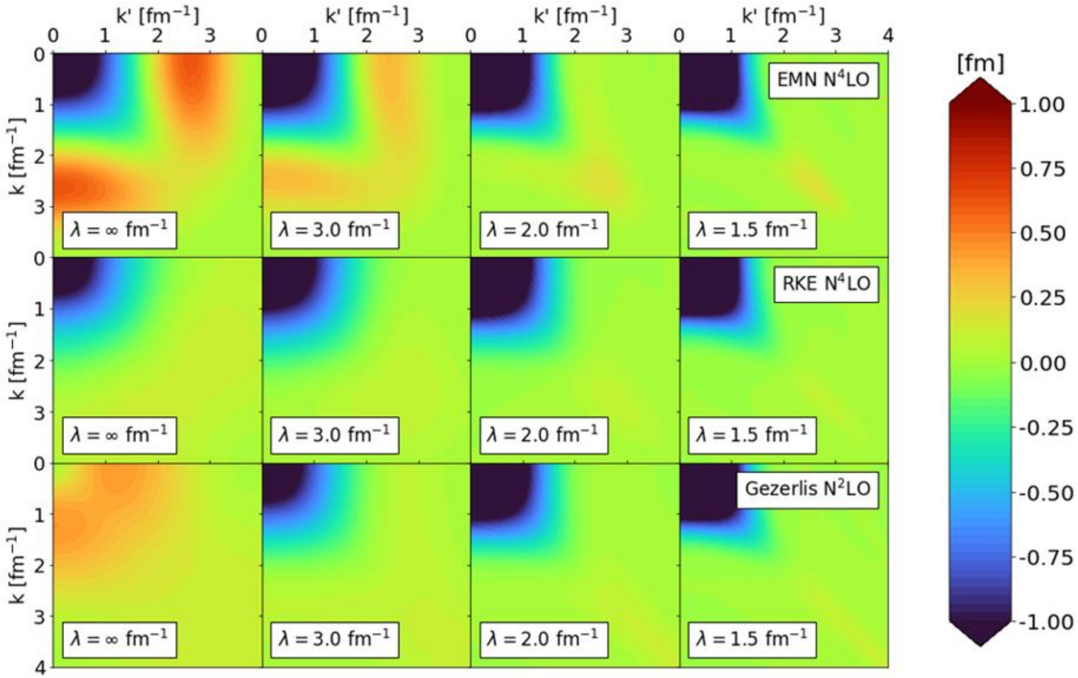
Results & Discussions

➢ **Universality of different chiral potentials**

EMN, $\mathrm{N}^4\mathrm{LO}$, non-local regulator, $\Lambda = 500$ MeV

RKE, $\mathrm{N}^4\mathrm{LO}$, local-non-local regulator, $\Lambda = 450$ MeV

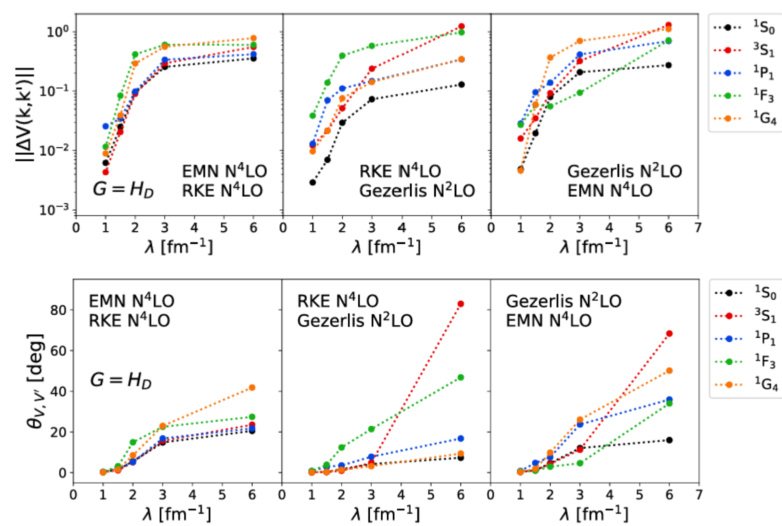
Gezerlis, $\mathrm{N}^2\mathrm{LO}$, local regulator, $\Lambda_\mathrm{r} = 1.0$ fm



* For the Wegner generator $G = H_D$

How to quantify the universality?

1. Frobenius norm of $\Delta V(k, k')$
2. Spectral distribution theory(SDT)



Results & Discussions

➢ **Universality of different chiral potentials**

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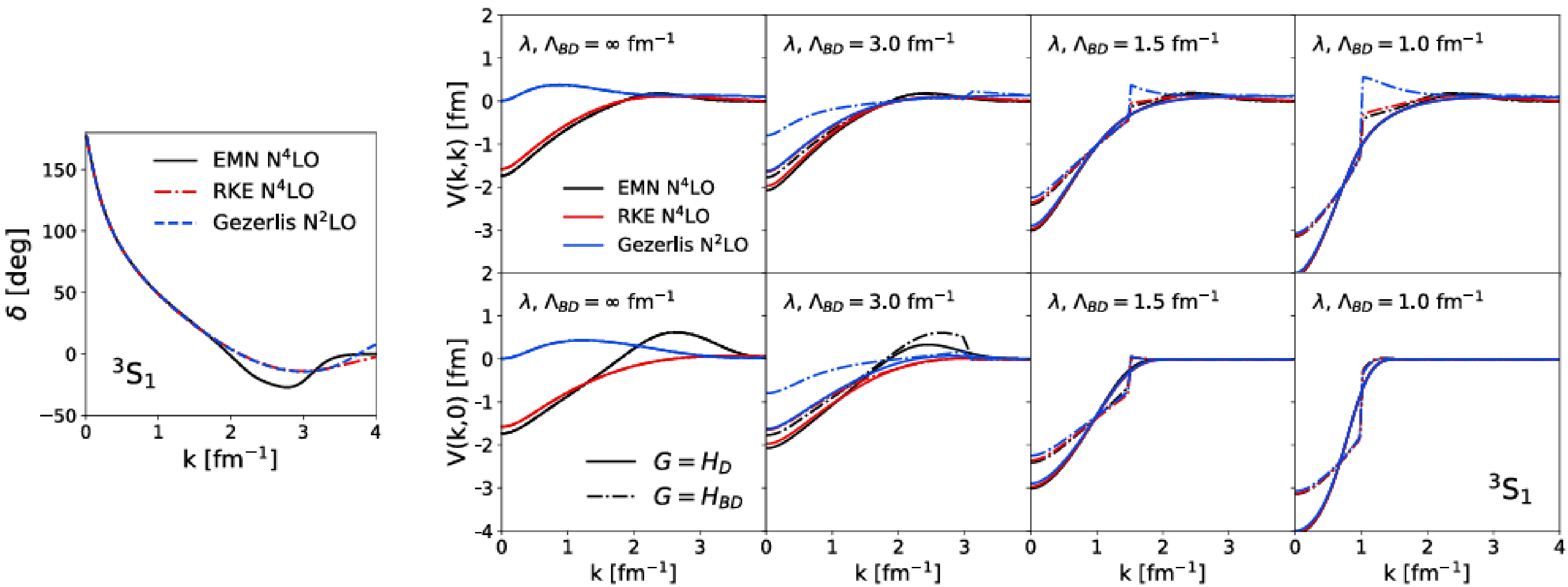
Gezerlis, $\mathrm{N^2LO}$, local regulator, $\Lambda_{\mathrm{r}} = 1.0$ fm

Comparison of the Wegner generator $G = H_D$ and the block-diagonal generator $G = H_{BD}$



(a) (b)

* For H_{BD} generators, λ is fixed at $1.0\ \mathrm{fm}^{-1}$.

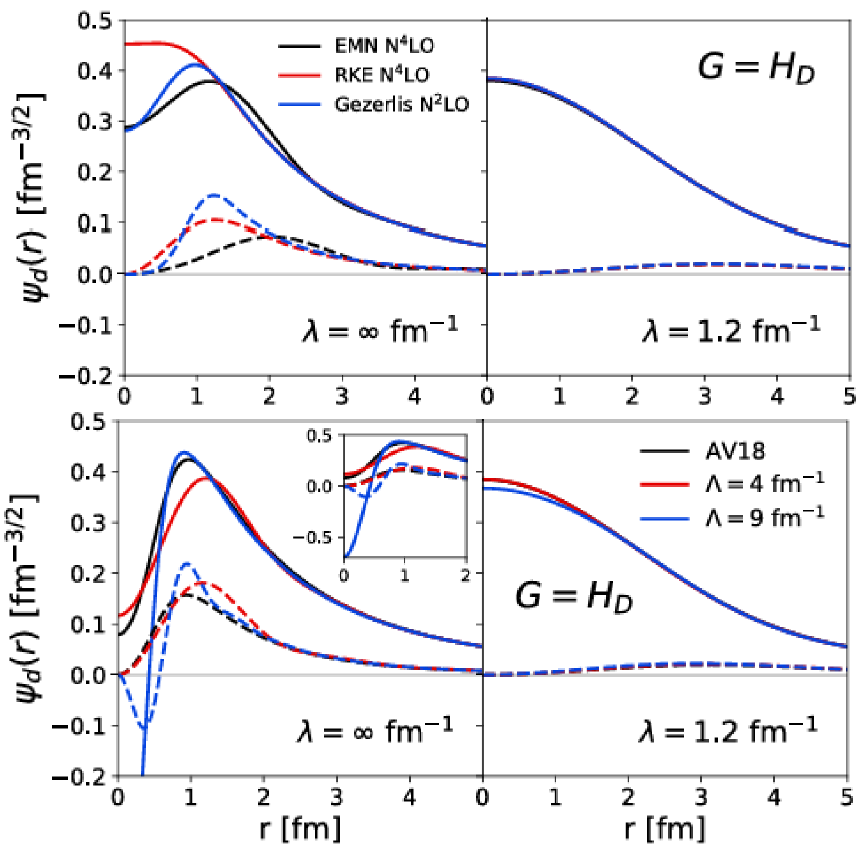
- **Universality of different chiral potentials**

EMN, $\mathrm{N^4LO}$, non-local regulator, $\Lambda = 500$ MeV

RKE, $\mathrm{N^4LO}$, local-non-local regulator, $\Lambda = 450$ MeV

Gezerlis, $\mathrm{N^2LO}$, local regulator, $\Lambda_\mathrm{r} = 1.0$ fm

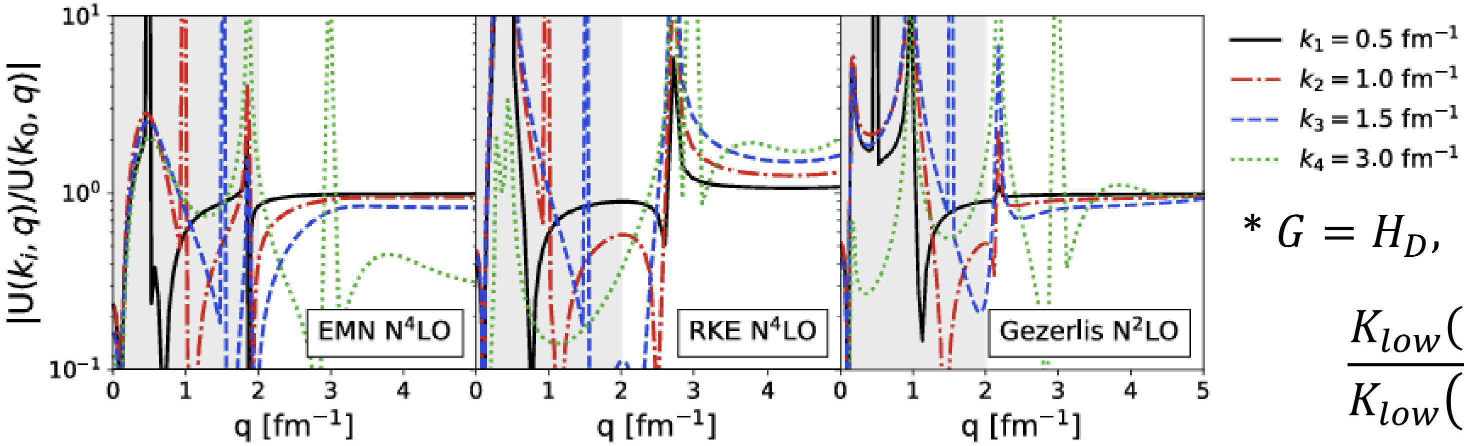
Comparison of the deuteron wave functions using the Wegner generator $G = H_D$



* The solid lines correspond to S state, and the dashed lines correspond to the D state.

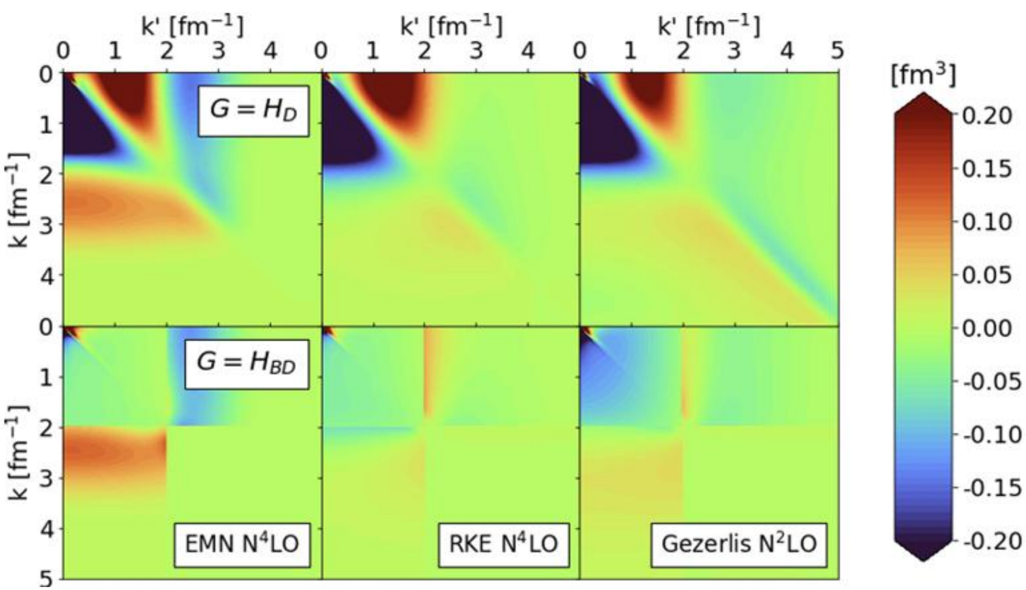
Results & Discussions

➢ **Factorization:** $U_\lambda(k,q) \to K_{low}(k)K_{high}(q) \propto K_{high}(q)$ **for** $k < \lambda \ll q$.



* $G = H_D,\ \lambda = 2\ \mathrm{fm}^{-1}$.

$$\frac{K_{low}(k_i)}{K_{low}(k_j)} \approx 1$$



* Matrix elements of
$\delta U(k,k') = U(k,k') - \mathbf{1}$

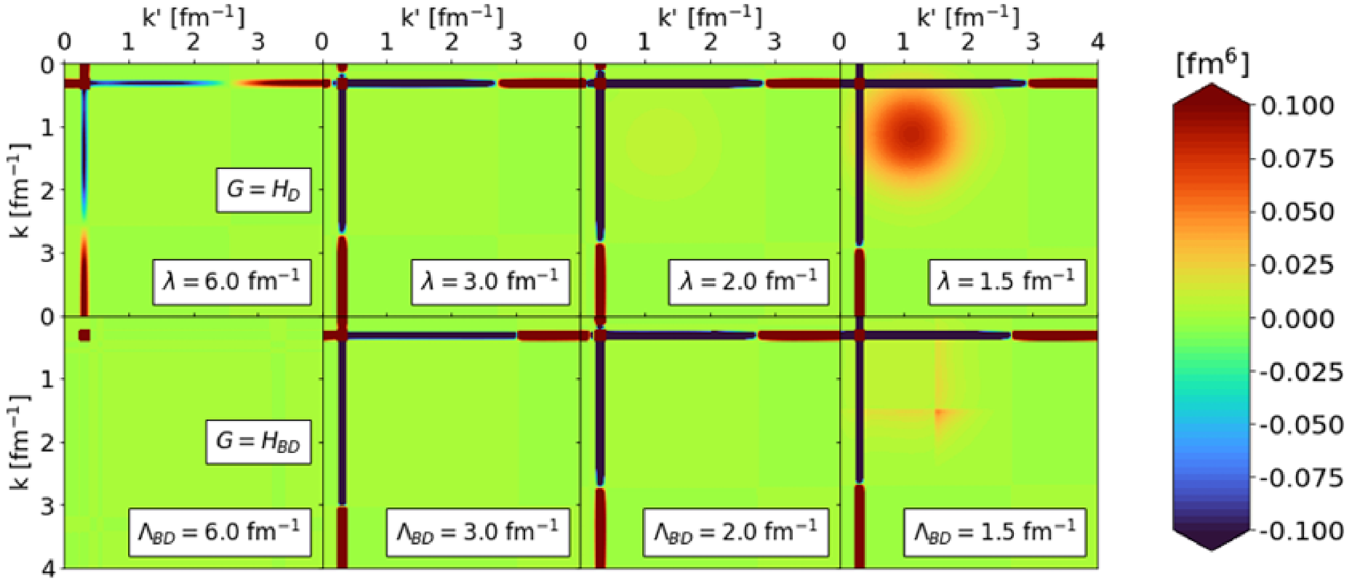
By fixing k' to a value much higher than λ or Λ_{BD} and see little variation in the ME.

High-momentum operators exhibit **universal scaling dependent only on the high-momentum physics** of the underlying NN potential.

Results & Discussions

➢ **Evolution of other operators**   * RKE, N^{4}LO, local-non-local regulator, $\Lambda = 450$ MeV

Operator $\boldsymbol{O}(\mathbf{0}) = \boldsymbol{a}_q^\dagger \boldsymbol{a}_q$, whose k, k' matrix element is proportional to $\delta(k-q)\delta(k'-q)$.



* Momentum projection operator $\left\langle k \left| a_q^\dagger a_q \right| k' \right\rangle$ for $q = 0.3\ \mathrm{fm}^{-1}$.

* For H_{BD} generators, λ is fixed at $1.0\ \mathrm{fm}^{-1}$.

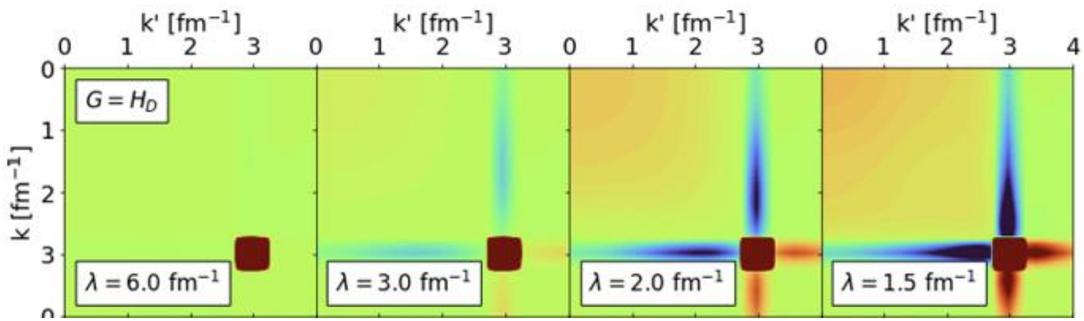
- ☐ The most evident induced contributions are nonzero bands for $k = q$ or $k = q'$, which is easy to understand by taking one step Δs in the SRG evolution $\frac{dO(s)}{ds} = [\eta(s), O(s)]$, which leads to $\left\langle k \left| \Delta a_q^\dagger a_q(s) \right| k' \right\rangle = \left\langle k \left| \left[\eta, a_q^\dagger a_q(0)\right] \right| k' \right\rangle \Delta s$.

- ☐ The Hamiltonian is being modified more by the band-diagonal evolution.

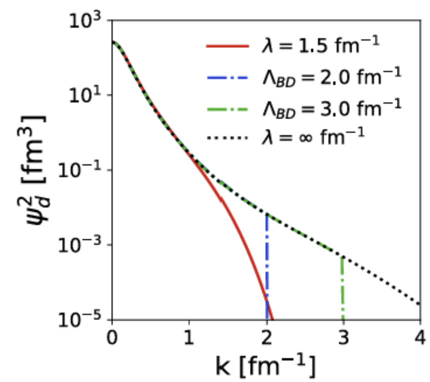
Results & Discussions

- **Evolution of other operators** * RKE, $\mathrm{N^4LO}$, local-non-local regulator, $\Lambda = 450$ MeV

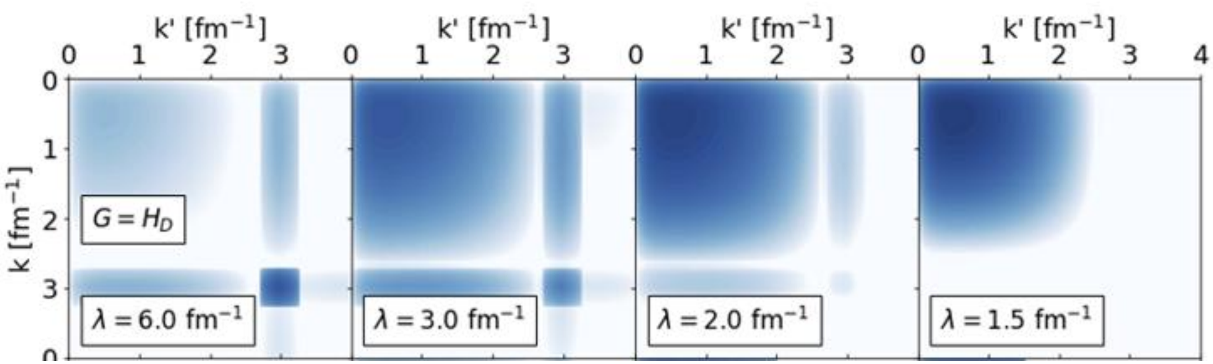
* Momentum projection operator $\left\langle k \left| a_q^\dagger a_q \right| k' \right\rangle$ for $q = 3\ \mathrm{fm}^{-1}$.



* Momentum distributions from deuteron.



* Integrand of $\left\langle \psi_d \left| a_q^\dagger a_q \right| \psi_d \right\rangle$ in momentum space.



Both the wave function and operator are SRG evolved so the total strength is preserved, i. e.,

$$\left\langle \psi_d(s) \left| a_q^\dagger a_q(s) \right| \psi_d(s) \right\rangle = \left\langle \psi_d(0) \left| a_q^\dagger a_q(0) \right| \psi_d(0) \right\rangle$$

Summary & Outlook

The Magnus expansion offers an improved variant of the standard SRG solution methods. And the flow equation of operators can be solved using simple, efficient methods.

Recently introduced chiral EFT Hamiltonians are characterized by a different type of scheme dependence in the use of qualitatively distinct regulators. In comparing their flows to low resolution, it is confirmed that **the momentum-space matrix elements of this new generation of chiral EFT Hamiltonians flow to a universal form** when **the decoupling scale is below the region of phase equivalence**.
This was examined quantitatively using **the Frobenius norm and SDT correlation coefficient** as measures of the differences in the evolved potentials.

By exploiting the **unitary invariance of measured observables**, we can shift the focus from **correcting many-body wave functions** to the **computationally simpler RG flow of the operators**.

Thank you for your attention!