# Operator evolution from the similarity renormalization group and the Magnus expansion

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## Abstract

Ideas for Magnus / SRG operator evolution paper

– SRG/Magnus evolution in different potentials (non-local, local, semi-local). Universality. High cutoffs.

– Block-diagonal generator for high cutoff potentials and operator evolution. How the block-diagonal generator handles spurious bound states.

– Testing the Magnus expansion for high cutoff potentials using the potentials from Wendt 2011 for comparison. Spurious bound states and connection to intruder states in IMSRG calculations.

– Operator evolution for different potentials and generators.

## I. INTRODUCTION

### NN interaction and SRG decoupling.

- Strong coupling between low- and high-momentum matrix elements in NN potentials.
- Very difficult to implement these interactions in many-body methods using basis expansions. Matrix dimension becomes too large for accurate calculations.
- RG transformations are used to soften the interaction to make many-body methods feasible. One such method, the SRG, also preserves observables from unitarity.

### SRG formalism

– The SRG decouples low- and high-momentum scales by applying a continuous unitary transformation $U(s)$ where $s = 0 \to \infty$ is the flow parameter.
– The 'dressed' or evolved operator is given by

$$O(s) = U(s)O(0)U^{\dagger}(s), \tag{1}$$

where $O(0)$ corresponds to the 'bare' operator.
– Because $U(s)$ is unitary, the observables of the operator are preserved.
– In practice, the unitary transformation U(s) is not explicitly solved for; the evolved operator is given by a differential flow equation which is obtained by taking the derivative of Eqn. (1),

$$\frac{dO(s)}{ds} = [\eta(s), O(s)], \tag{2}$$

where $\eta(s) = \frac{dU(s)}{ds}U^{\dagger}(s) = -\eta^{\dagger}(s)$ is the anti-hermitian SRG generator.
– The generator is defined as a commutator, $\eta(s) = [G, H(s)]$, where $G$ specifies the type of flow or form of the decoupled operator.
– By setting $G = H_D(s)$, the diagonal of the Hamiltonian, the operator is driven to band-diagonal form.
– This choice was implemented by Wegner in condensed matter physics [1].
– In a similar option used in nuclear physics, $G$ is set to the relative kinetic energy, $T_{rel}$, which also drives to band-diagonal form.
– It is convenient to define $\lambda \equiv s^{-1/4}$ which roughly measures the width of the band-diagonal in the decoupled operator.

– For block-diagonal decoupling, denoted $G = H_{BD}(s)$, the operator is split into low- and high-momentum sub-blocks by specifying a separation in momentum $\Lambda_{BD}$.
– These transformations are similar to $V_{lowk}$ Lee-Suzuki transformations but keep the high-momentum matrix elements non-zero, although entirely decoupled from the low-momentum sub-block.
– Generally the flow equation (2) is solved up to some finite value of $s$ with a high-order ODE solver.
– For notational convenience, we write the generators without the $s$ dependence in the rest of the paper.

**Background on modern nuclear potentials.**

– Wide range of NN potentials.

- Chiral EFT background.
- Different potentials but give same $S$-matrix.
- How do different potentials change under SRG transformations?

**Universality**

– The explicit long-range physics should be the same. Decoupling low- and high-energy gives matching low-energy matrix elements. In the NN potential, this means softened NN interactions should have the same low-momentum matrix elements after sufficient decoupling.
– Add takeaways from Dainton: phase shift equivalence implies matrix element equivalence for $\lambda$ approaching the momenta of phase equivalence. Correct binding energy is critical or the lowest matrix elements will not match.
– Motivate long list of unaddressed questions: regulator, generator dependence, high cutoffs, the Magnus expansion.

- Regulator. Functional dependence of regulator. Reasons for implementing each.
- Generators. Band- and block-diagonal transformations.
- High cutoffs. Cite Nogga, Wendt, and Tews papers.
- The Magnus expansion. High cutoffs and connection to IMSRG intruder state problem.

**Operator evolution**

– State how a potential and wave function changes: how does this affect other operators?

– Operator evolution for different potentials (regulators, chiral order, etc.)

– How operators evolve from band- and block-diagonal SRG transformations.

**Overview of sections.**

## II. SRG EVOLUTION OF NN POTENTIALS

**General outline of the section**

– Comparison of potential evolution with different regulators, orders, generators.

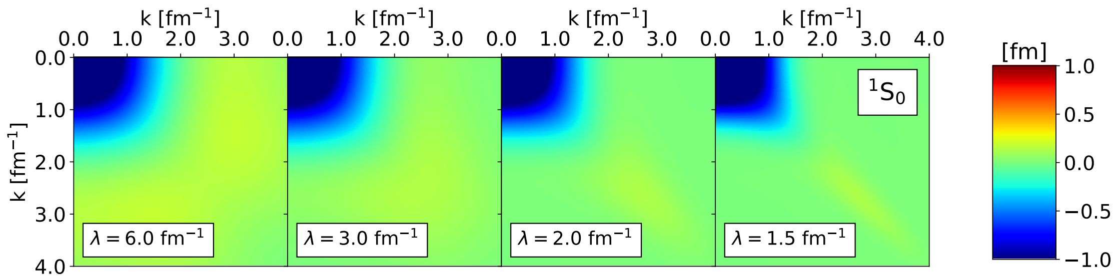
– Universality.

– Discussion of high cutoffs, block-diagonal generator at high cutoffs, and how it handles spurious bound states.

– Use high cutoffs to transition to Magnus test problem.

**Analysis of figures**

– Fig. 1 illustrates the SRG in a nutshell. Here, we evolve three partial wave channels of RKE $N^3LO$ [2] where the cutoff $\Lambda = 450$ MeV to $\lambda = 1.5$ $\text{fm}^{-1}$. We see that the off-diagonal elements of the potential approach zero and the potential is driven to band-diagonal form.

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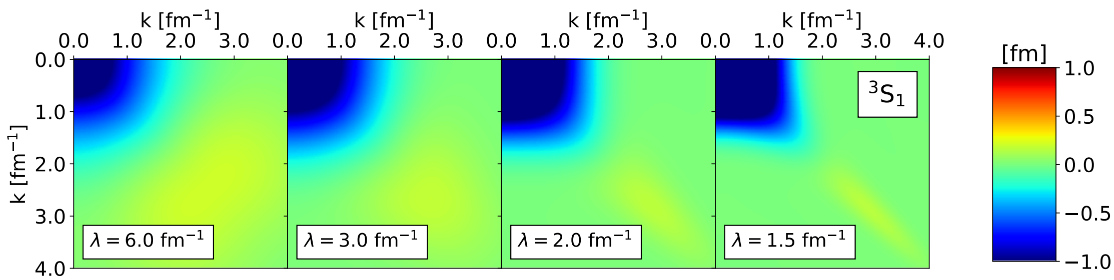


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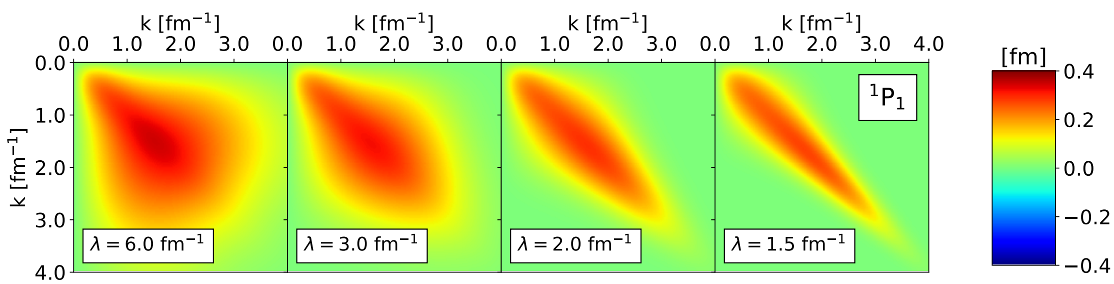
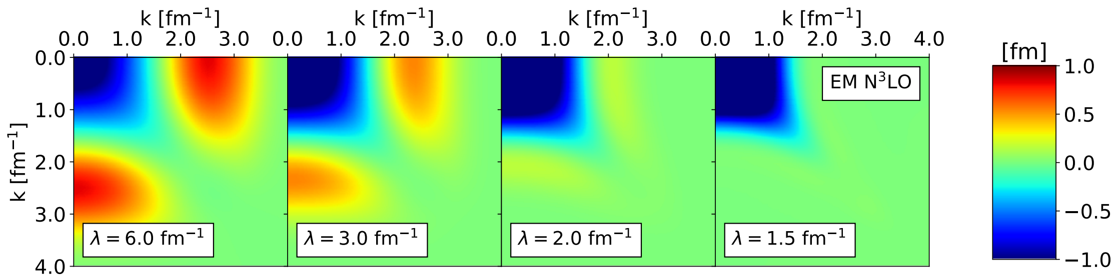



(c)

FIG. 1: Matrix elements of the RKE N$^3$LO potential SRG-evolving in $\lambda$ right to left under transformations with the Wegner generator in the $^1$S$_0$ (a), $^3$S$_1$ (b), and $^1$P$_1$ (c) channels.

– In Fig. 2 we consider three different SRG-evolved potentials in the $^3$S$_1$ channel: EM N$^3$LO (500 MeV cutoff) [3], RKE N$^3$LO (450 MeV cutoff) [2], and Gezerlis et al. N$^2$LO (1 fm cutoff) [4]. The major difference in these three potentials are the regulator functions in the contact and pion-exchange terms. The EM N$^3$LO interaction is a non-local potential where both contact and pion-exchange interactions feature a non-local regulator function of the form $\exp[-(p/\Lambda)^{2n} - (p'/\Lambda)^{2n}]$, where $\Lambda$ is the momentum-space cutoff and $n$ is an integer. However, a non-local regulator function for pion-exchange contributions can introduce regulator artifacts for cutoffs $\Lambda$ lower than the breakdown scale $\Lambda_b$. Several semi-local chiral potentials have been introduced to reduce regulator artifacts, such as the RKE $N^3LO$ potential. Here, a local regulator function is applied for the long-range interactions in momentum-space, while a non-local regulator function is used for the short-range interactions. In some instances, non-local interactions are not suitable for *ab initio* approaches such as the quantum Monte Carlo (QMC) method motivating the need for fully local potentials. The Gezerlis et al. $N^2LO$ potential is an example of a local interaction where the long-range terms have a local regulator function in coordinate-space and the short-range terms have a local regulator function in momentum-space.

– Takeaways from Fig. 2: completely different at $\lambda = 6$ fm$^{-1}$ but low-momentum matrix elements are similar at $\lambda = 1$ fm$^{-1}$. Decoupled, low-momentum matrix elements are necessarily the same since the pion-exchange terms are calculated explicitly. (Cutoff dependence can play a role though for lower cutoffs.)

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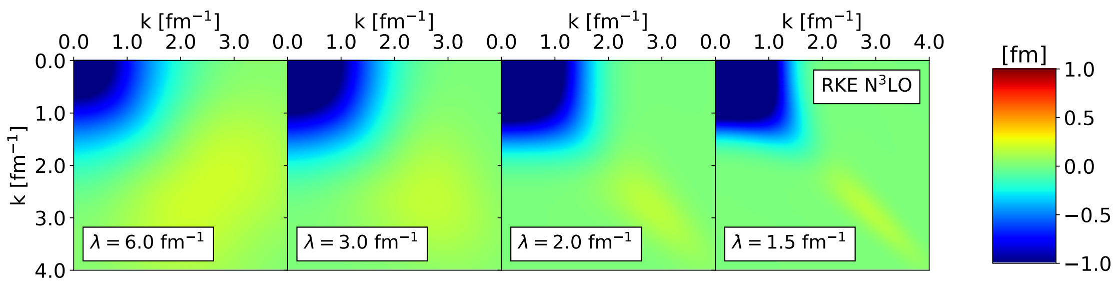


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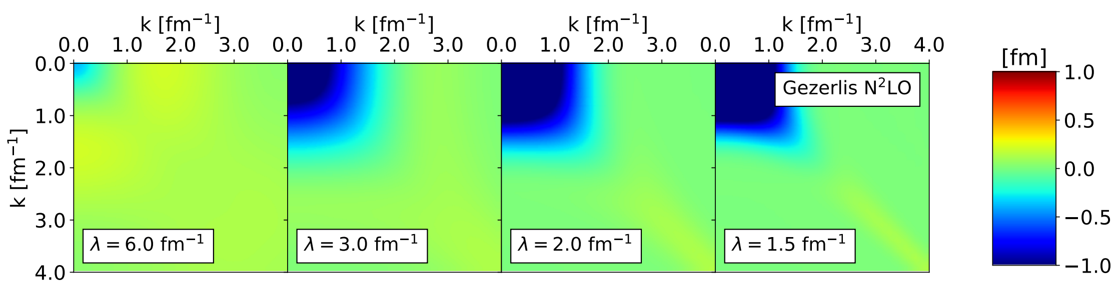


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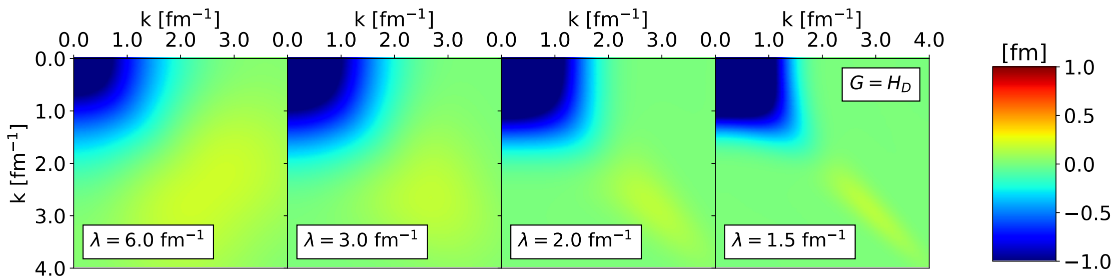
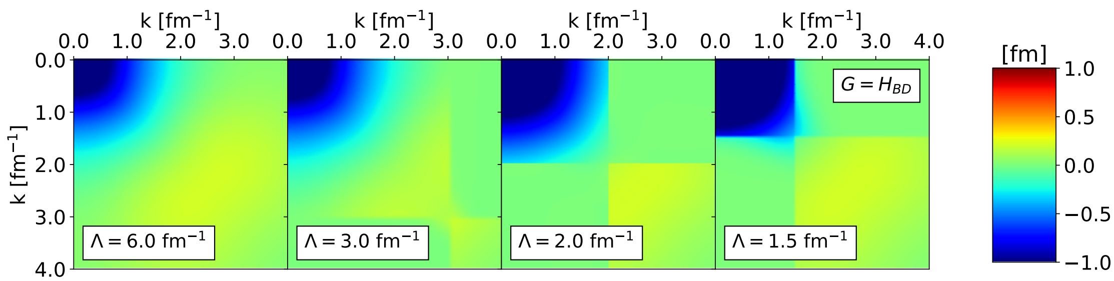
FIG. 2: Matrix elements of the EM N$^3$LO (a), RKE N$^3$LO (b), and Gezerlis et al. N$^2$LO (c) potentials SRG-evolving in $\lambda$ right to left under transformations with the Wegner generator in the $^3$S$_1$ channel.

– Fig. 3 shows the SRG-evolved RKE N$^3$LO (450 MeV cutoff) potential in the $^3$S$_1$ channel for two SRG generators: the Wegner and block-diagonal generators which drive the potential to band- and block-diagonal form, respectively. We continue to evolve to band-diagonal form with respect to the parameter $\lambda$, but for the block-diagonal generator, we label sub-plots with the parameter $\Lambda$ which characterizes the sharp cutoff in decoupling the low- and high-momentum matrix elements.

– Takeaways from Fig. 3: smooth decoupling for Wegner and sharp for block-diagonal, each unique generator should have its own type of universality. Check this more quantitatively by comparing matrix element "slices".




(a)



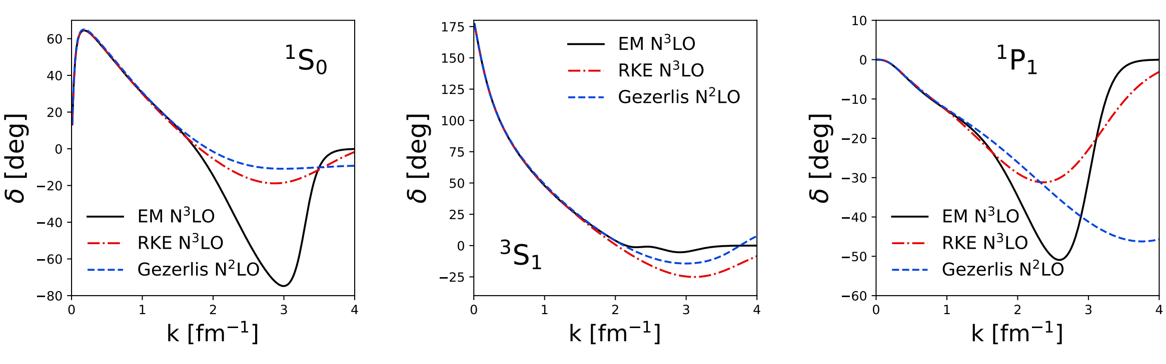

(b)

FIG. 3: Matrix elements of the RKE N$^3$LO potential SRG-evolving right to left under transformations with Wegner (a) and block-diagonal (b) generators in the $^3$S$_1$ channel. Here, we use $\lambda$ for Wegner evolution in the top row and $\Lambda$ for block-diagonal evolution in the bottom row. For block-diagonal evolution, we fix $\lambda = 1.5$ fm$^{-1}$.

– Fig. 4 shows the NN phase shifts of EM N$^3$LO, RKE N$^3$LO, and Gezerlis et al. N$^2$LO potentials in the $^1$S$_0$, $^3$S$_1$, and $^1$P$_1$ channels. In [5], it was found that phase equivalence up to some value of momentum $k$ implies matrix element equivalence up to the same value of $k$ in SRG-evolved potentials. We verify this conclusion by checking the matrix elements in Fig. 5 where we see a collapse of the different potential matrix elements to the same line in the last column ($\lambda = 1$ fm$^{-1}$). Note, Figs. 5-7 show both Wegner and block-diagonal evolution where the solid lines correspond to the Wegner generator and dash-dotted to block-diagonal evolution. We see each generator collapses the potential to a different form because the low- and high-momentum matrix elements decouple in a different manner.

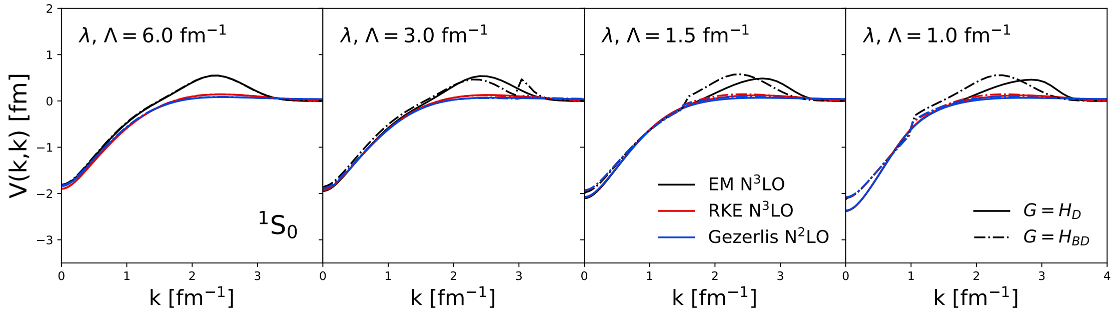
– In the $^3$S$_1$ channel, we see a slight deviation in the lowest momentum potential matrix element from EM N$^3$LO and the other two potentials. This is due to a minor difference in the deuteron binding energy ($\approx 1\%$ difference).

– The bottom row of Fig. 7 shows $V(k, 0.5)$ instead of $V(k, 0)$ because the far off-diagonal matrix elements in the $^1$P$_1$ channel are all zero.




(a) (b) (c)

FIG. 4: $^1$S$_0$ (a), $^3$S$_1$ (b), and $^1$P$_1$ (c) phase shifts for the EM N$^3$LO (solid black), RKE N$^3$LO (red dash-dotted), and Gezerlis et al. N$^2$LO (blue dashed) potentials.

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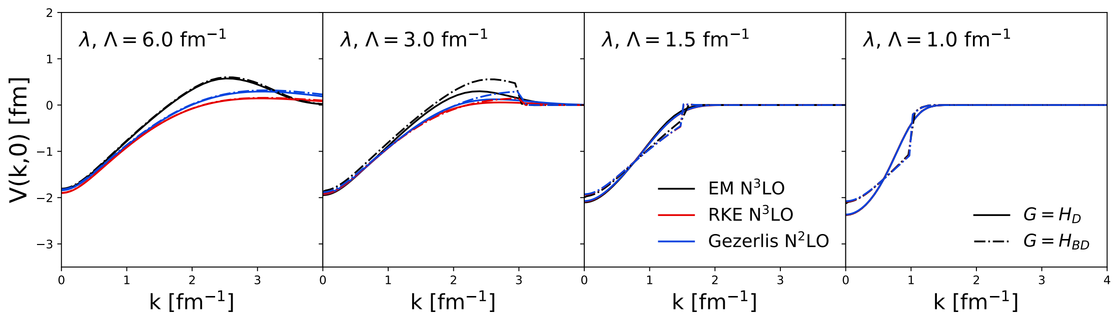
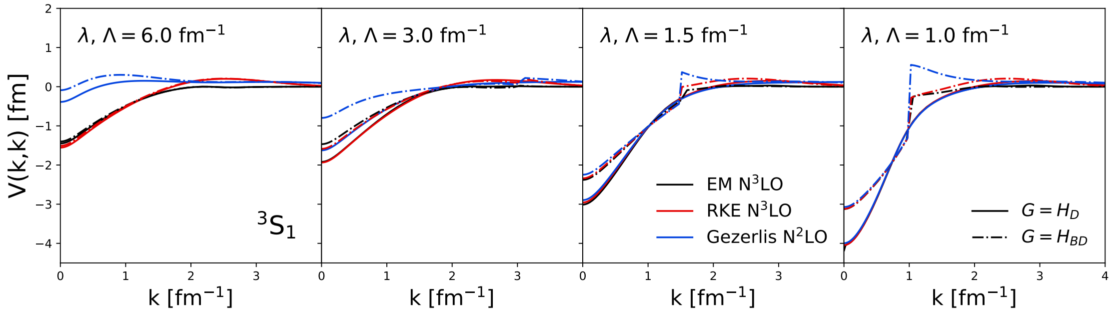



(b)

FIG. 5: Diagonal (a) and far off-diagonal (b) matrix elements of the EM N$^3$LO (black), RKE N$^3$LO (red) and Gezerlis et al. N$^2$LO (blue) potentials SRG-evolving right to left under transformations with Wegner (solid) and block-diagonal (dash-dotted) generators in the $^1$S$_0$ channel. Here, we use $\lambda$ for Wegner evolution and $\Lambda$ for block-diagonal evolution. For block-diagonal evolution, we fix $\lambda = 1$ fm$^{-1}$.

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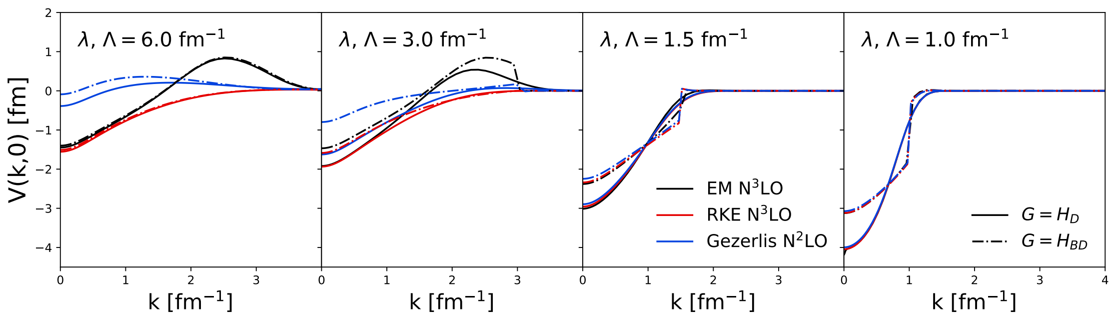


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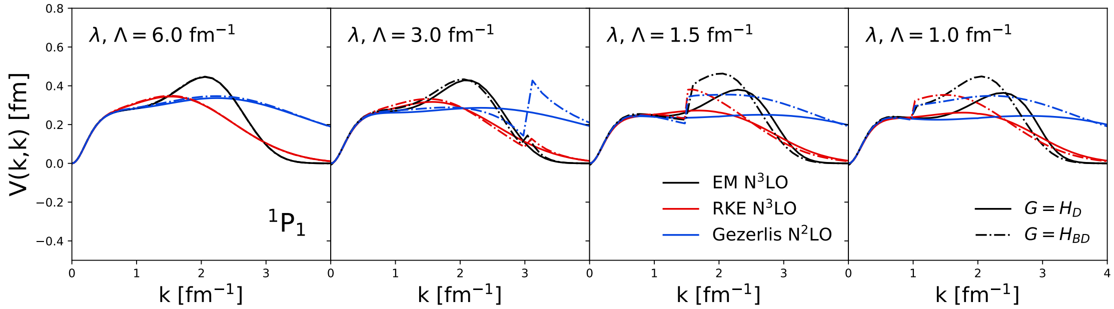
FIG. 6: Same as Fig. 5 but in the $^3S_1$ channel.

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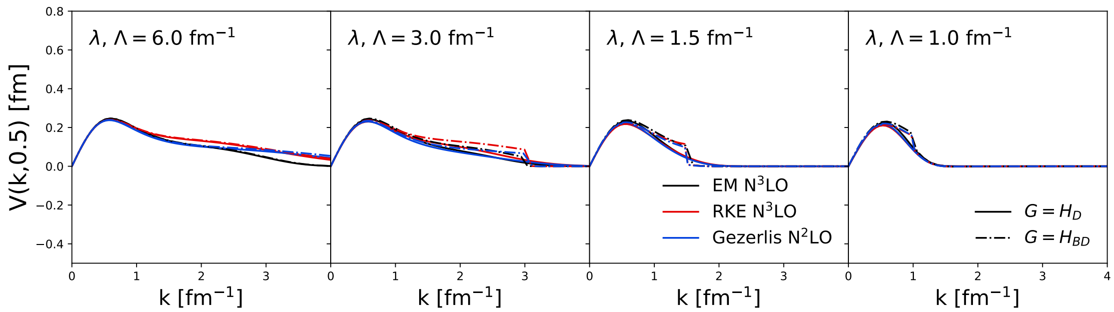
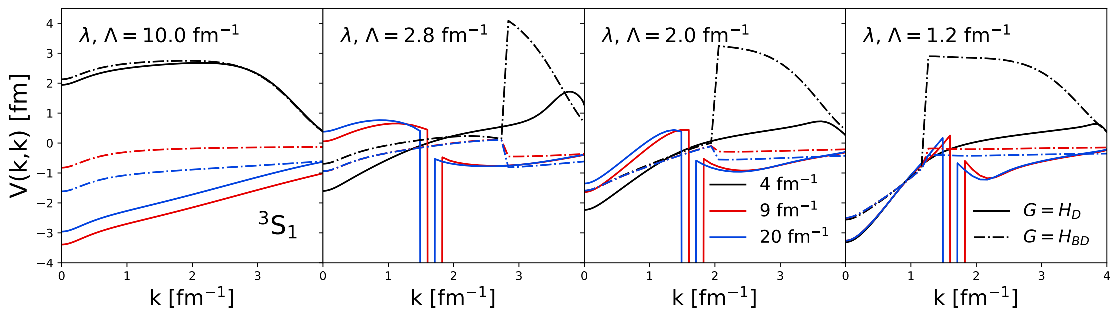



(b)

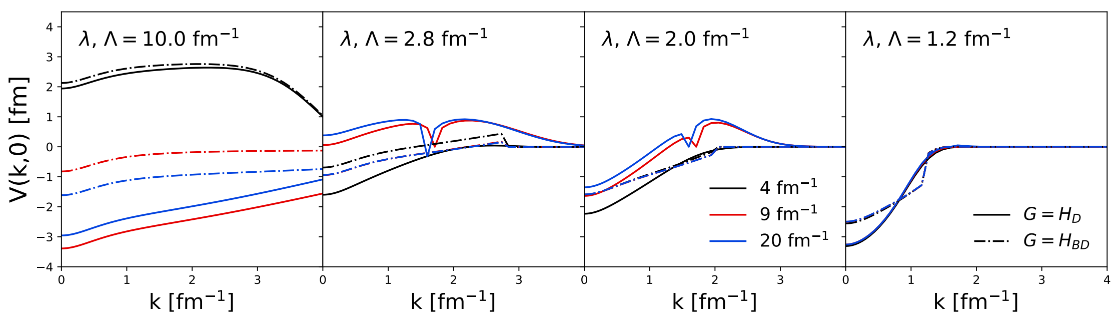
FIG. 7: Same as Figs. 5 and 6 but in the $^1$P$_1$ channel.

## High cutoffs

- Cutoff dependence in non-local LO (Wendt) potential.
- Band- and block-diagonal evolution and universality. Add figure analogous to Fig. 6 but for $\Lambda = 4$, 9, and 20 fm$^{-1}$.
- Spurious bound state(s).
- Discussion on how the block-diagonal generator handles spurious bound states. Where they are "decoupled" in the matrix compared to Wegner.
- Transition to Magnus expansion.




(a)




(b)

FIG. 8: Diagonal (a) and far off-diagonal (b) matrix elements of the non-local LO potentials at cutoffs $\Lambda = 4$ (black), 9 (red) and 20 (blue) $\mathrm{fm}^{-1}$ SRG-evolving right to left under transformations with Wegner (solid) and block-diagonal (dash-dotted) generators in the $^3\mathrm{S}_1$ channel. Here, we use $\lambda$ for Wegner evolution and $\Lambda$ for block-diagonal evolution. For block-diagonal evolution, we fix $\lambda = 1.2\ \mathrm{fm}^{-1}$.

## III. THE MAGNUS EXPANSION

– Connection to IMSRG intruder state.

### A. Formalism

– Motivation: simplifies computational problem for evolving multiple operators, exact unitarity.

– We now consider the Magnus implementation.

– Mathematically speaking, the Magnus expansion is a method for solving an initial value problem associated with a linear ordinary differential equation (ODE).

– Formal details of the Magnus expansion are discussed in [6].

– We will introduce the Magnus expansion in the context of SRG evolving any operator.

– In an intermediate step in deriving Eqn. (2), we have a linear ODE for $U(s)$,

$$\frac{dU(s)}{ds} = \eta(s)U(s). \tag{3}$$

– Magnus showed that one can solve the following equation with a solution $U(s) = e^{\Omega(s)}$ where $\Omega(s)$ is expanded as a power series, $\sum_n^\infty \Omega_n$ (referred to as the Magnus expansion or Magnus series).

– The terms of the series are given by integral expressions involving $\eta(s)$ (again, see [6, 7] for details).

– For our case, we focus on the formally exact derivative of $\Omega(s)$,

$$\frac{d\Omega(s)}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_\Omega^k(\eta), \tag{4}$$

where $B_k$ are the Bernoulli numbers, $ad_\Omega^0(\eta) = \eta(s)$, and $ad_\Omega^k(\eta) = [\Omega(s), ad_\Omega^{k-1}(\eta)]$.

– We integrate this differential equation to find $\Omega(s)$ and evaluate the unitary transformation directly.

– Then the evolved operator can be evaluated with the BCH formula:

$$O(s) = e^{\Omega(s)} O e^{-\Omega(s)} = \sum_{k=0}^{\infty} \frac{1}{k!} ad_\Omega^k(O). \tag{5}$$

– As $k \to \infty$ in both sums in Eqns. (4) and (5) the Magnus transformation matches the SRG transformation exactly.

– We investigate several truncations $k_{max}$ in Eqn. (4) and take many terms, $k_{max} \sim 25$, in Eqn. (5).

– Here or earlier (for the following bullets)? Better to motivate the Magnus in the introduction or easier to explain given mathematical detail?

– There are significant advantages in the Magnus implementation.

– In the typical approach, the numerical error associated with solving the flow equation affects the accuracy of the observables for the evolved operator.

– Therefore, one must use a high-order ODE solver in integrating the flow equation (2).

– In the Magnus implementation, unitarity is guaranteed by the form of $U(s)$; in fact, one could solve Eqn. (4) with a simple first-order Euler step-method keeping the same observables while decoupling the operator as desired.

– This offers a decent computational speed-up by avoiding a high-order solver.

– In this paper, we demonstrate this advantage by applying the Magnus implementation using the first-order Euler step-method.

– The second major advantage involves the evolution of multiple operators.

– In many other situations, one may be interested in evolving several operators at a time.

– In the SRG procedure, we would have another set of coupled equations in Eqn. (2), drastically increasing memory usage.

– Each additional operator increases the set of equations - say $N$ equations - by another factor of $N$.

– In the Magnus, one only needs $\Omega(s)$ to consistently evolve several operators.

– We avoid the cost in memory by directly constructing $U(s) = e^{\Omega(s)}$.

– This is especially useful in IMSRG calculations where the model space can be very large.

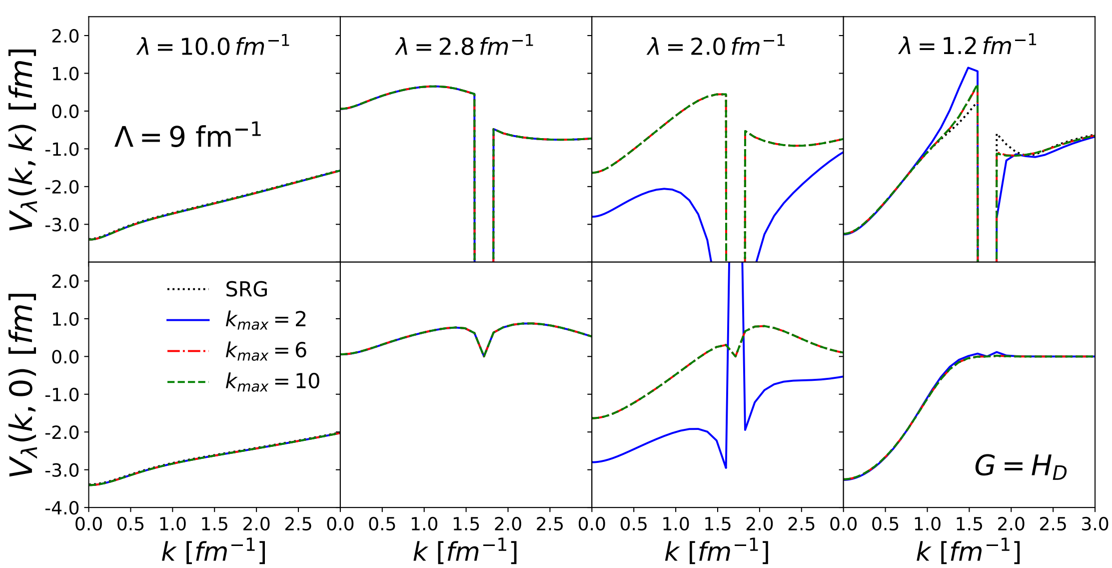
– In the next section, we discuss results from Magnus-evolved large-cutoff potentials focusing on the flow of the potential, observables, and operator evolution.

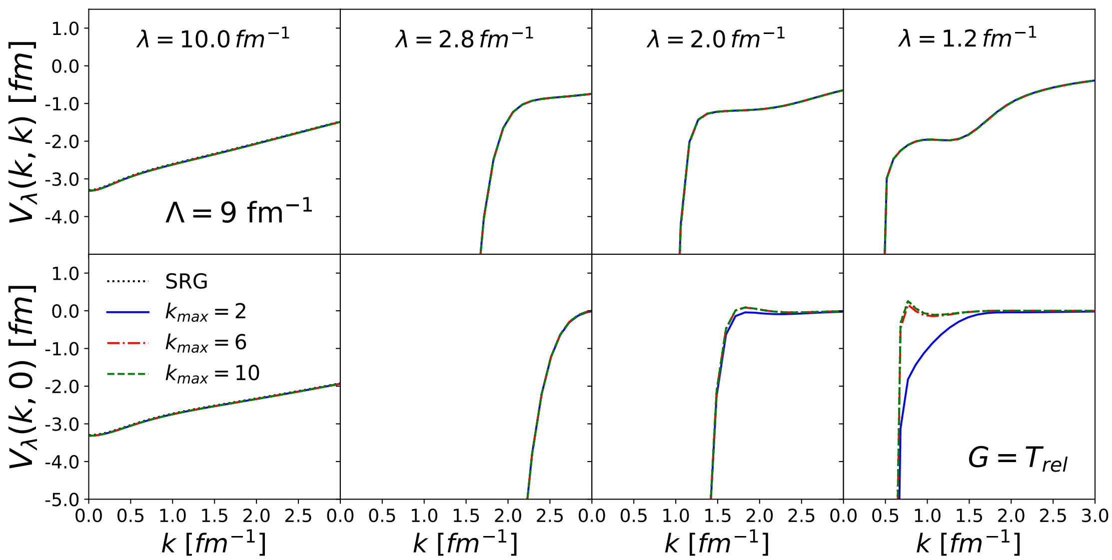
### B. Results

– Comparison to Wendt problem.

– Implications for IMSRG.

– Use discussion of operator evolution to transition to next section.






## IV. EVOLUTION OF OTHER OPERATORS

– SRG operator evolution for different potentials and generators.

– General questions to address: universality for operators, different generators.

– Momentum projection operator.

- Contours and general behavior: SRG transformation shifts strength of operator to low-momentum.

- Deuteron momentum distributions. Why does this make sense with the transformed operators?

- Diagonals and far off-diagonals. Universality.

- Same questions but with figures of the integrand.

– Note, the unitary transformations and evolved wave functions for different potentials are not the same (at low momentum too) swhich implies that evolved operators cannot have the same universality property as the evolved potentials since they are dependent on the evolved wave functions.

– $\hat{r}^2$ operator.

## V. CONCLUSION

– Summary.

– Outlook.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