

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

Background on modern nuclear potentials.

- Wide range of NN potentials.
 - Chiral EFT background.
 - Different potential matrix elements but give same S -matrix.
- Implementation to many-body calculations and SRG decoupling.
 - Strong coupling between low- and high-momentum matrix elements in realistic 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.
 - How do different interactions change under SRG transformations?

SRG formalism

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

$$O(s) = U(s)O(0)U^\dagger(s), \quad (1)$$

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),

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

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.

- To drive the operator to band-diagonal form, set $G = H_D(s)$, the diagonal of the Hamiltonian.
- 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 Λ_{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.

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 λ 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.

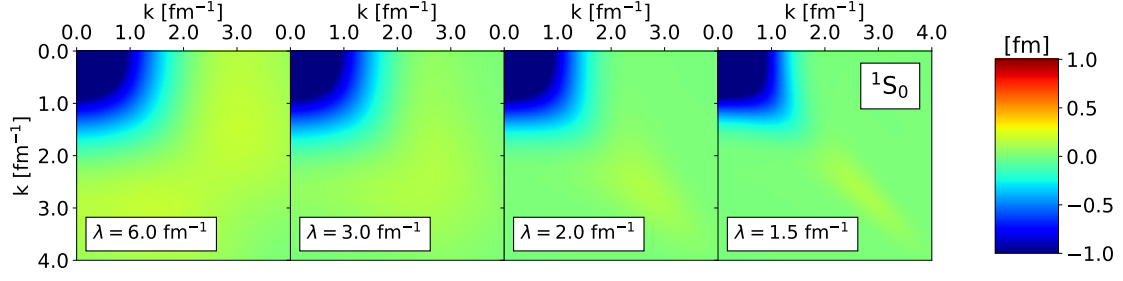
Operator evolution

- 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.

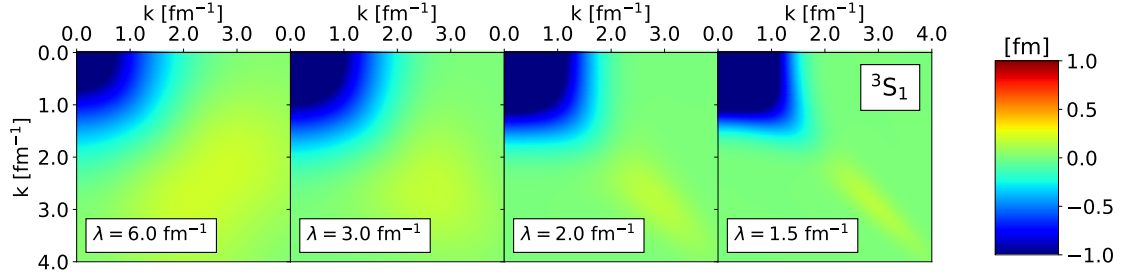
Overview of sections.

II. SRG EVOLUTION OF NN POTENTIALS

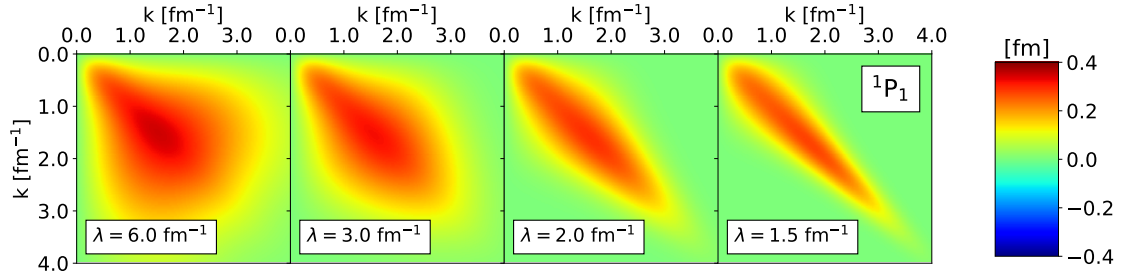
- Comparison of potential evolution with different regulators, orders, generators.
- Universality.
- Discussion of high cutoffs, block-diagonal generator at high cutoffs, and how it handles spurious bound states.
- Use high cutoffs to transition to Magnus test problem.



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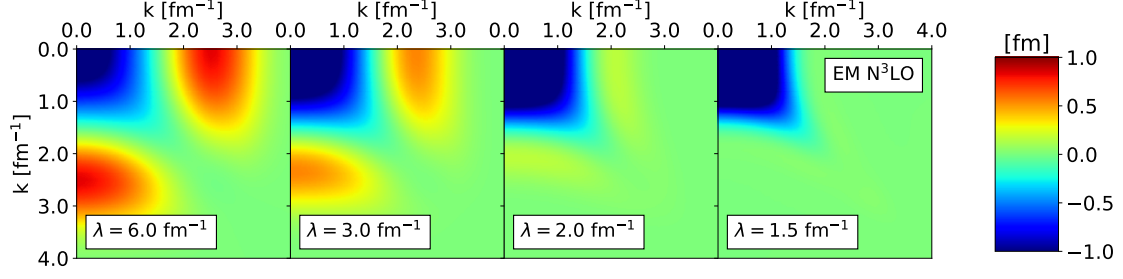


(b)

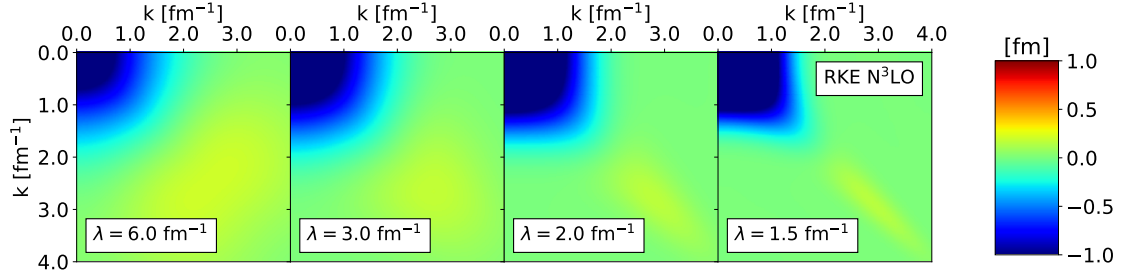


(c)

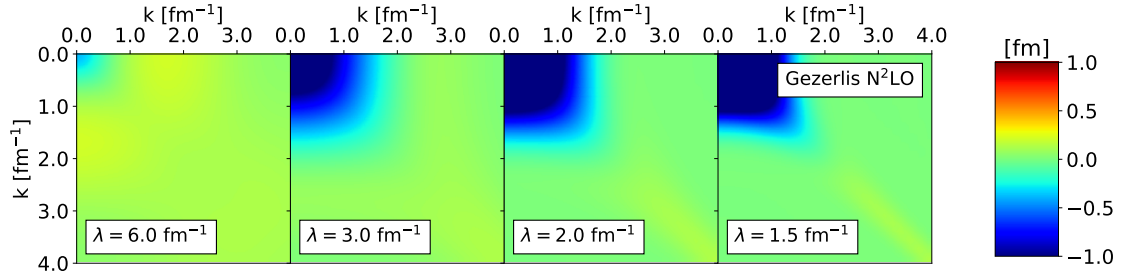
FIG. 1: Matrix elements of the RKE $N^3\text{LO}$ potential SRG-evolving in λ right to left under transformations with the Wegner generator in the 1S_0 (a), 3S_1 (b), and 1P_1 (c) channels.



(a)



(b)



(c)

FIG. 2: Matrix elements of the EM N³LO (a), RKE N³LO (b), and Gezerlis et al. N²LO (c) potentials SRG-evolving in λ right to left under transformations with the Wegner generator in the 3S_1 channel.

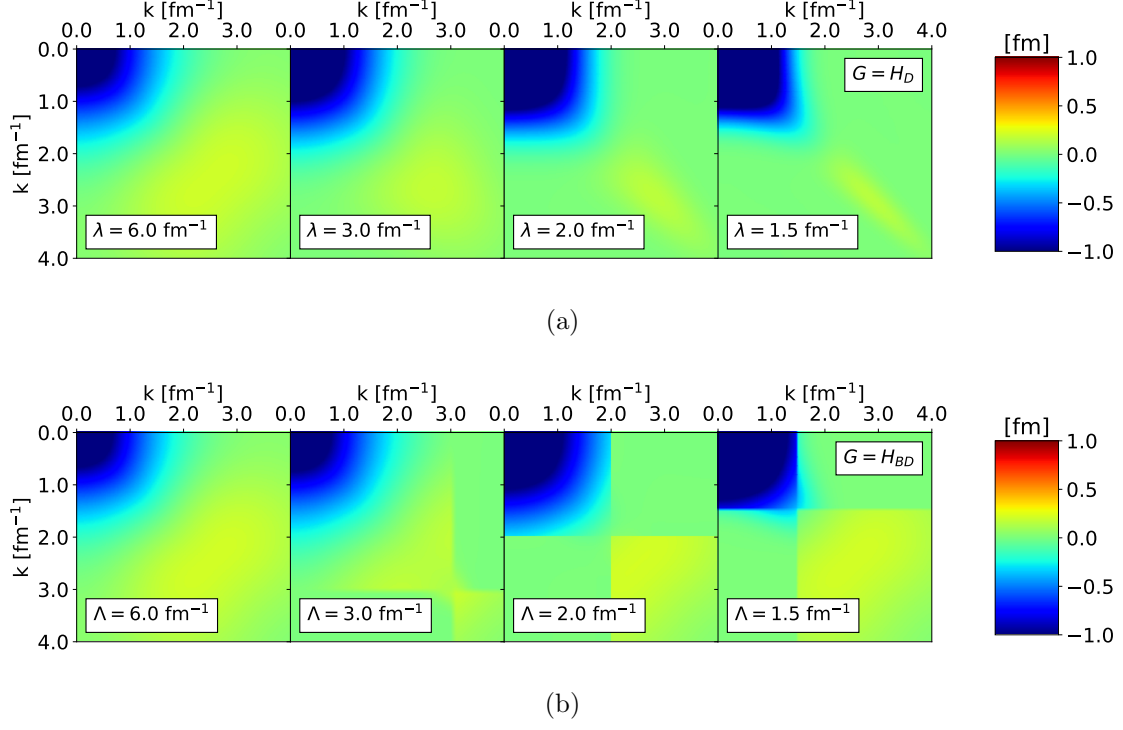


FIG. 3: Matrix elements of the RKE N³LO potential SRG-evolving right to left under transformations with Wegner (a) and block-diagonal (b) generators in the ³S₁ channel. Here, we use λ for Wegner evolution in the top row and Λ for block-diagonal evolution in the bottom row. For block-diagonal evolution, we fix $\lambda = 1.5 \text{ fm}^{-1}$.

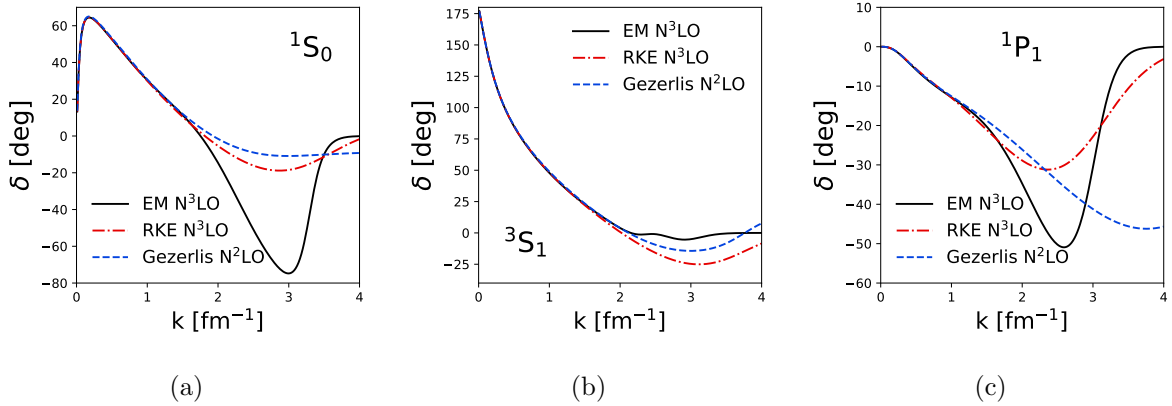
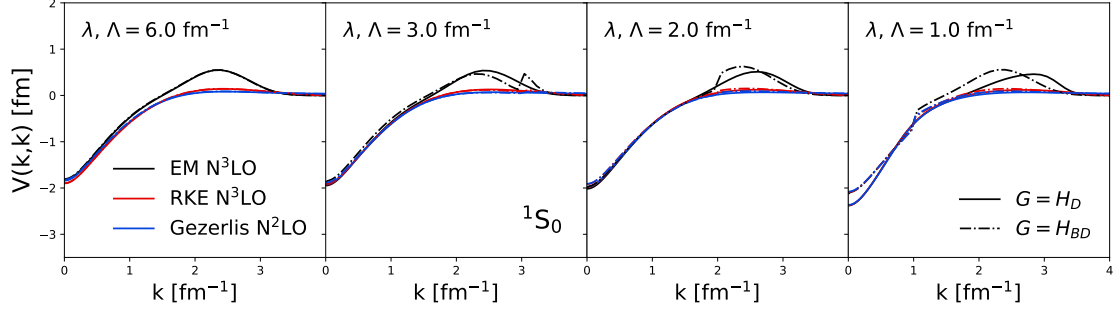
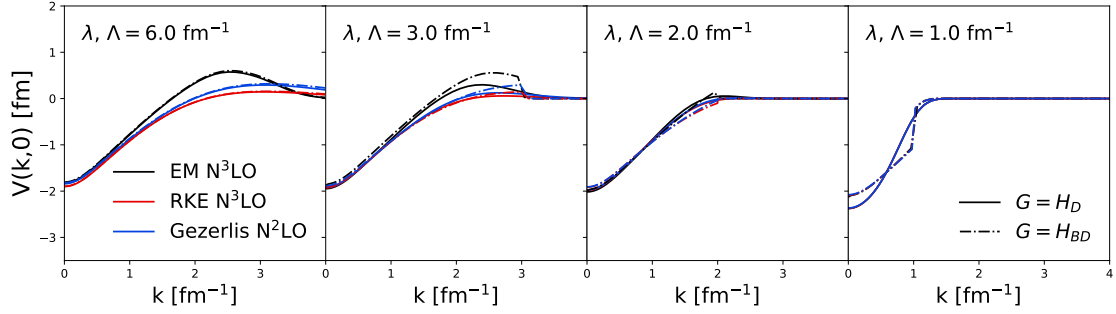


FIG. 4: ¹S₀ (a), ³S₁ (b), and ¹P₁ (c) phase shifts for the EM N³LO (solid black), RKE N³LO (red dash-dotted), and Gezerlis et al. N²LO (blue dashed) potentials.

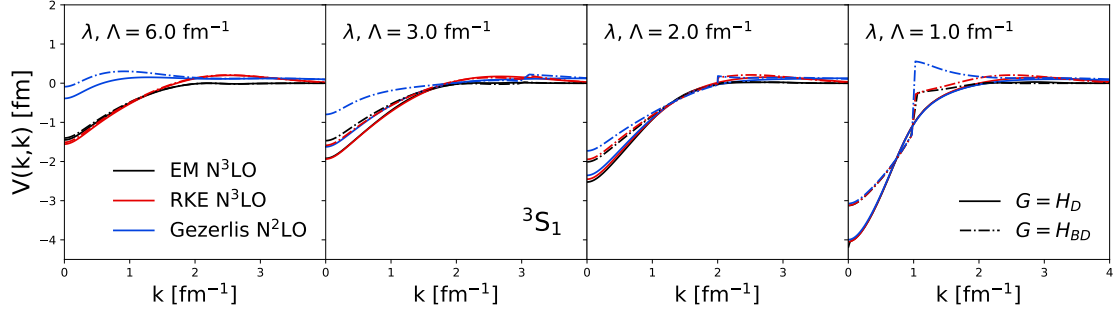


(a)

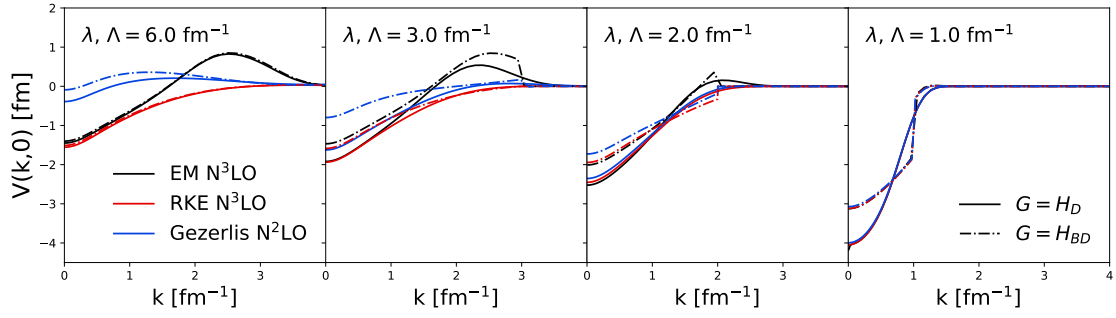


(b)

FIG. 5: Diagonal (a) and far off-diagonal (b) matrix elements of the EM N³LO (black), RKE N³LO (red) and Gezerlis et al. N²LO (blue) potentials SRG-evolving right to left under transformations with Wegner (solid) and block-diagonal (dash-dotted) generators in the ¹S₀ channel. Here, we use λ for Wegner evolution and Λ for block-diagonal evolution. For block-diagonal evolution, we fix $\lambda = 1.0 \text{ fm}^{-1}$.



(a)



(b)

FIG. 6: Same as Fig. ?? but in the 3S_1 channel.

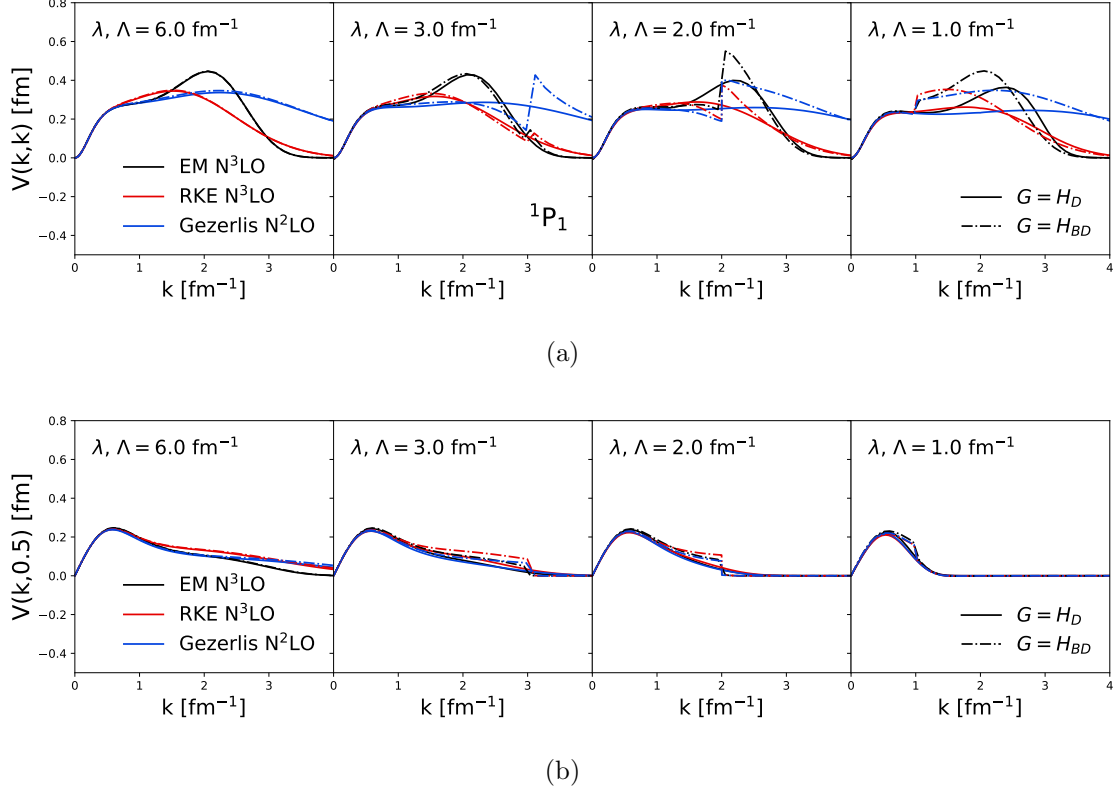


FIG. 7: Same as Figs. ?? and ?? but in the 1P_1 channel.

III. THE MAGNUS EXPANSION

- Summary of Wendt high cutoff results and 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 [?].
- 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 $U(s)$,

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

- 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, $\sum_n \Omega_n$ (referred to as the Magnus expansion or Magnus series).
- The terms of the series are given by integral expressions involving $\eta(s)$ (again, see [? ?] for details).
- For our case, we focus on the formally exact derivative of $\Omega(s)$,

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

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:

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

- As $k \rightarrow \infty$ 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.

A. Building SRG unitary transformations

Diagonalize initial and evolved Hamiltonians which we will call $H(0)$ and $H(s)$, respectively. This gives $\psi_\alpha(0)$ and $\psi_\alpha(s)$ for each eigenvalue indexed by α . Then the SRG unitary transformation can be computed by taking a sum over outer products of the evolved and initial wave functions:

$$U(s) = \sum_{\alpha=1}^N |\psi_\alpha(s)\rangle \langle \psi_\alpha(0)|, \quad (6)$$

where N is the dimension of the Hamiltonian matrix. Here the weights are factored into the wave functions, thus $U(s)$ is unitless.

To evolve operators, we simply apply $U(s)$:

$$O(s) = U(s)O(0)U^\dagger(s), \quad (7)$$

where $O(0)$ is the bare operator.

B. Momentum projection operator: $a_q^\dagger a_q(k, k')$

Applying $a_q^\dagger a_q(k, k')$ to a wave function $\psi(k)$ returns $\psi(q)$. For the discrete case, $\psi(k_i)$ is an $N \times 1$ vector and $a_q^\dagger a_q(k_i, k_j)$ is an $N \times N$ matrix where $i, j = 1 \cdots N$. Then $a_q^\dagger a_q(k, k')$ acting on $\psi(k)$ is a matrix multiplication, implying a continuous integration over $d^3k/(2\pi)^3 = 2/(\pi k^2 dk)$ in spherical coordinates. Therefore, we include a factor of $\pi/(2k_i k_j \sqrt{w_i w_j})$ in $a_q^\dagger a_q(k_i, k_j)$ where w represents the momentum weights. In matrix form,

$$a_q^\dagger a_q(k_i, k_j) = \frac{\pi \delta_{k_i q} \delta_{k_j q}}{2k_i k_j \sqrt{w_i w_j}}, \quad (8)$$

which has units fm^3 . To evolve operators, we apply $U(s)$ at this point. For mesh-independent figures, we must divide by an additional factor of $k_i k_j \sqrt{w_i w_j}$. This operator is inherently mesh-dependent based off discretizing $\delta_{k_i q} \delta_{k_j q}$ above.

C. Momentum distribution function: $\phi^2(k)$

We diagonalize the Hamiltonian for eigenvectors ψ_α . In the $^3\text{S}_1$ - $^3\text{D}_1$ coupled channel, the S-component is given by $\psi_\alpha[:N]$ and the D-component by $\psi_\alpha[N:]$ where N is the length of the momentum mesh. Then the momentum distribution of the state α is given by,

$$|\phi_\alpha(k)|^2 = |\psi_\alpha[:N]|^2 + |\psi_\alpha[N:]|^2. \quad (9)$$

This satisfies the normalization condition $\sum_{i=1}^N |\phi(k_i)|^2 = 1$, implying that the factor $k^2 dk$ (or in the discrete case, $k_i^2 w_i$) is factored into the wave function. For mesh-independent figures, divide by $k_i^2 w_i$.

V. CONCLUSION

- Summary.
- Outlook.

[1] F. Wegner, *Annalen der Physik* **506**, 77 (1994).