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.

– Variety of potentials.

– Implementation to many-body calculations and SRG decoupling.

– Regulators, order, cutoff, etc. Universality.

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,

$$\eta(s) = [G, H(s)], \tag{3}$$

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].

– For notational convenience, we write the Wegner choice without the s dependence in the rest of the paper.

– 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.

– In this paper, we consider both choices.

– Add block-diagonal generator.

– Generally the flow equation (2) is solved up to some finite value of s with a high-order ODE solver.

– It is convenient to define $\lambda \equiv s^{-1/4}$ which roughly measures the width of the band-diagonal in the decoupled operator.

Operator evolution

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

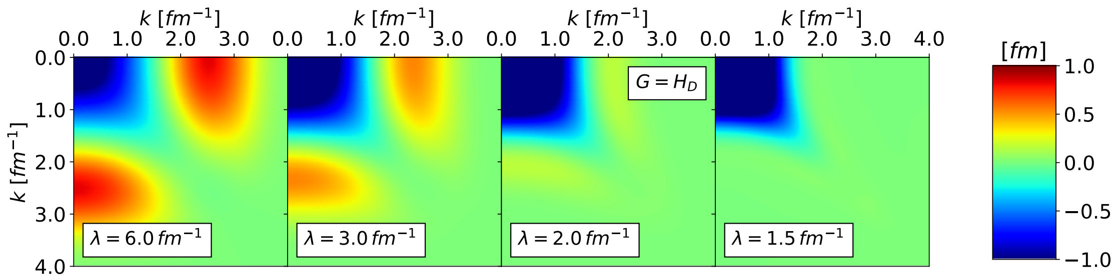
– How operators evolve from band- and block-diagonal SRG transformations.

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

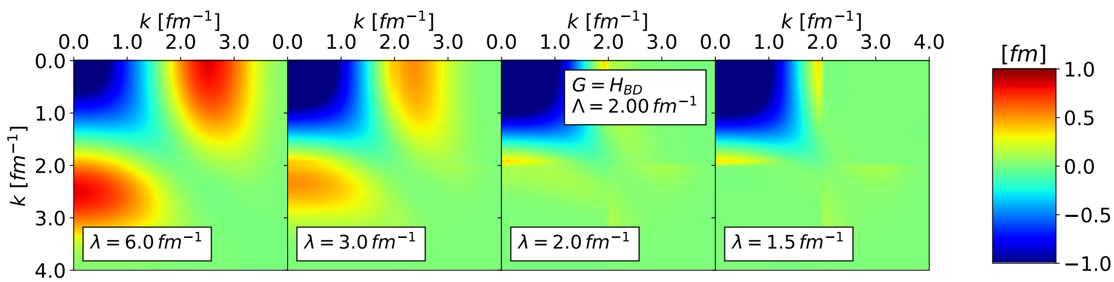
– Mention the Magnus expansion?

II. SRG EVOLUTION OF NN POTENTIALS

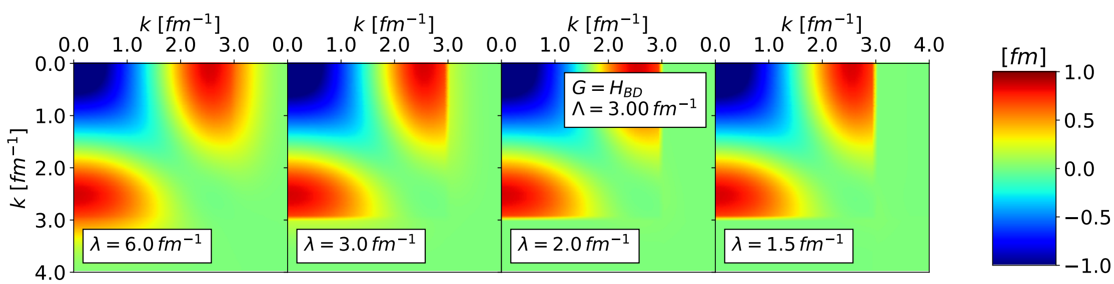
– Example figure. EM N^{3}LO potential.



(a)



(b)



(c)

FIG. 1: Matrix elements of the Entem-Machleidt N^{3}LO non-local potential $V_\lambda(k, k')$ SRG-evolving in λ right to left under transformations with the Wegner generator (a) and block-diagonal generators decoupling at $\Lambda = 2$ and 3 fm^{-1} (b and c).

III. THE MAGNUS EXPANSION

A. Formalism

– 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 $U(s)$,

$$\frac{dU(s)}{ds} = \eta(s)U(s). \tag{4}$$

– 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 [**? ?**] for details).

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

$$\frac{d\Omega(s)}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_\Omega^k(\eta), \tag{5}$$

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:

$$O(s) = e^{\Omega(s)} O e^{-\Omega(s)} = \sum_{k=0}^{\infty} \frac{1}{k!} ad_\Omega^k(O). \tag{6}$$

– As $k \to \infty$ in both sums in Eqns. (5) and (6) the Magnus transformation matches the SRG transformation exactly.

– We investigate several truncations k_{max} in Eqn. (5) and take many terms, $k_{max} \sim 25$, in Eqn. (6).

– 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. (5) 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.

IV. EVOLUTION OF OTHER OPERATORS

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:

$$U(s) = \sum_{\alpha=1}^{N} |\psi_\alpha(s)\rangle \langle\psi_\alpha(0)| \,, \tag{7}$$

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 $U(s)$:

$$O(s) = U(s)O(0)U^\dagger(s), \tag{8}$$

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,

$$a_q^\dagger a_q(k_i,k_j) = \frac{\pi \delta_{k_i q}\delta_{k_j q}}{2k_i k_j\sqrt{w_i w_j}}, \tag{9}$$

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 ${}^3S_1$-${}^3D_1$ 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,

$$|\phi_\alpha(k)|^2 = |\psi_\alpha[:N]|^2 + |\psi_\alpha[N:]|^2. \tag{10}$$

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).