Decoupling of bound states with the Magnus expansion and the IMSRG

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Abstract

The in-medium similarity renormalization group (IMSRG) softens nucleon-nucleon interactions by applying a continuous unitary transformation to the Hamiltonian to decouple low- and high-energy scales. We study differences between evolving nuclear Hamiltonians with the typical SRG approach and with the Magnus expansion implementation by applying these approaches to a leading-order nucleon-nucleon potential in momentum space that features a spurious, deeply bound state at higher χ^{EFT} cutoffs. We find that the Magnus implementation converges to the typical SRG approach.

Introduction

- Nuclear structure calculations are complicated by coupling of the ground state to excitations
- IMSRG solves the nuclear many-body problem by decoupling the ground state from particle/hole excitations
- "Rotate" the Hamiltonian with continuous unitary transformation $U(s)$

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

- Evolve Hamiltonian via flow equation:

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

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

where G specifies the type of flow

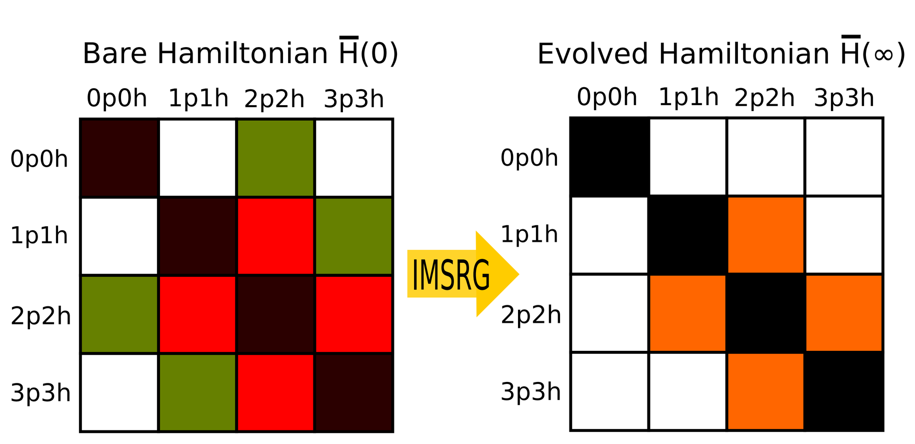

Figure 1: Hamiltonian in the many-body basis evolved with an IMSRG transformation

The Magnus Expansion

- Transformation of the form $U(s) = e^{\Omega(s)}$ exists
- Solve for $\Omega(s)$ which give $U(s)$ directly:

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

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

- Directly solving for $U(s)$ allows us to evolve *any* operator, not just H (e.g. electromagnetic transitions and moments)
- $U(s)$ is unitary regardless of the error on $\Omega(s)$
  - Eigenvalues of evolved operator are preserved
  - No need for high-order ODE solver - use first-order Euler method

$$\Omega_{n+1}(s) = \Omega_n(s) + \frac{d\Omega(s)}{ds} ds \tag{5}$$

  - No loss in accuracy in observables despite crude method
- Modest computational speed-up and substantial memory savings when solving for several operators

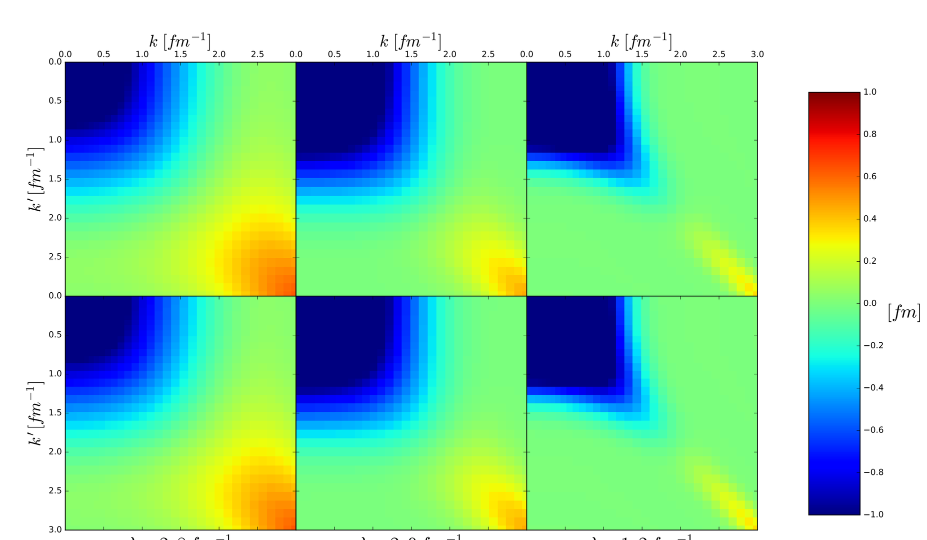

Figure 2: Contour of SRG evolved $V_\lambda(k, k')$ with $\Lambda = 4.0\, fm^{-1}$, $G = T_{rel}$ (top) and $G = H_D$ (bottom) for several values of $\lambda = s^{-1/4}$

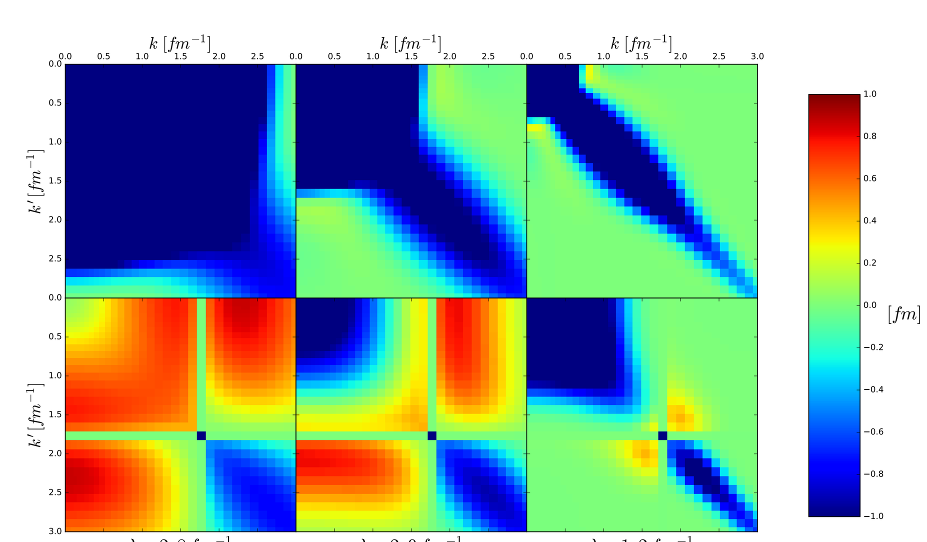

Figure 3: Contour of SRG evolved $V_\lambda(k, k')$ with $\Lambda = 9.0\, fm^{-1}$, $G = T_{rel}$ (top) and $G = H_D$ (bottom) for several values of λ

χ^{EFT} at High Cutoffs

- χ^{EFT} is the underlying theory for nucleon-nucleon interactions
  - Effective field theory (EFT) comprised of proton, neutron, and pion degrees of freedom
  - Requires a regularization procedure to separate high- and low-energy physics (the separation in energy scales is denoted by Λ)
- At high cutoffs ($\Lambda \sim 9$ fm^{-1}) nuclear potentials produce spurious, deeply bound states
- Spurious bound states can distort SRG evolution depending on choice of G (see Fig. 3)
  - $G = T_{rel}$: spurious bound state distorts the low-momentum block of $H(s)$
  - $G = H_D$: keeps spurious bound state safely outside low-momentum block
  - E.g., deuteron wave function at low-momentum is significantly affected by the spurious bound state with T_{rel} but not with H_D
- Apply the Magnus implementation on this difficult test case where evolution is sensitive to choice in G

Results

Comparison of Magnus to SRG evolution

- Low truncation in the Magnus expansion gives undesirable evolution
- Magnus converges to SRG result around $k \sim 4$
- Evolution of spurious bound state matches the SRG result regardless of truncation on Magnus expansion

Accuracy of observables

- $U(s)$ is a unitary transformation and should preserve observables
- Relative error of deuteron binding energy: $\delta\epsilon_d = |\frac{\epsilon_d - \tilde{\epsilon}_d}{\epsilon_d}|$ where $\tilde{\epsilon}_d$ corresponds to evolved Hamiltonian
- SRG: $\delta\epsilon_d \sim 10^{-6}$ (compounds error in solving ODE)
- Magnus: $\delta\epsilon_d \sim 10^{-13}$

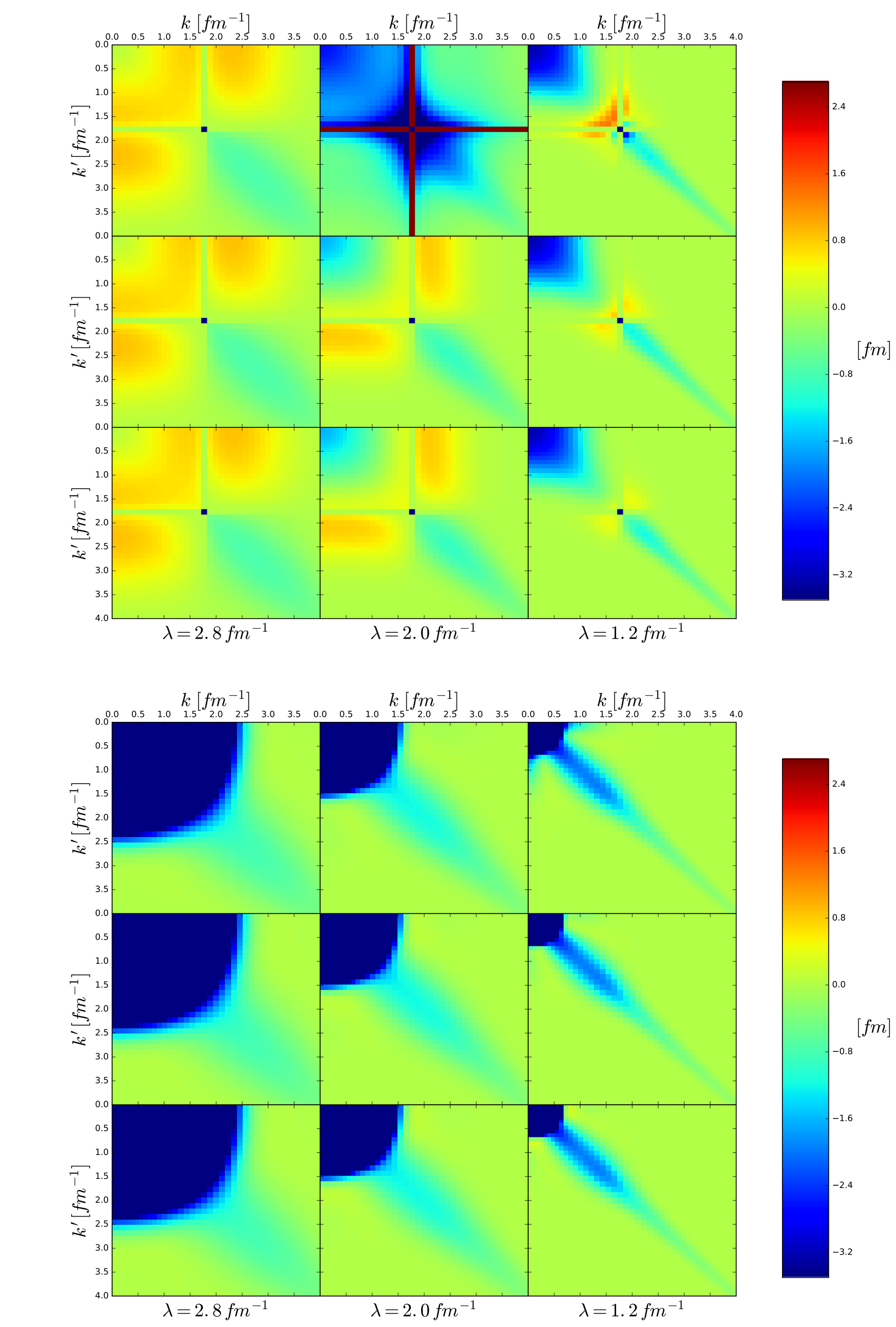

Figure 4: Contour of evolved $V_\lambda(k, k')$ with $\Lambda = 9.0\, fm^{-1}$, $G = H_D$ (top figure) and $G = T_{rel}$ (bottom figure) for several values of λ with each row corresponding to a different truncation in the Magnus expansion or the SRG result (2, 4, SRG)

Conclusion

- Magnus expansion improves viability/efficiency of the SRG
- Magnus implementation matches SRG H_D and T_{rel} evolution (given high enough truncation)
- Does the sensitivity to choice of generator carry over to Magnus/IMSRG calculations?
- How does the decoupling of spurious bound state(s) depend on Λ and regulator?

References

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