Decoupling of bound states with the Magnus expansion and the IM-SRG

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NUCLEI

Nuclear Computational Low-Energy Initiative

NSF

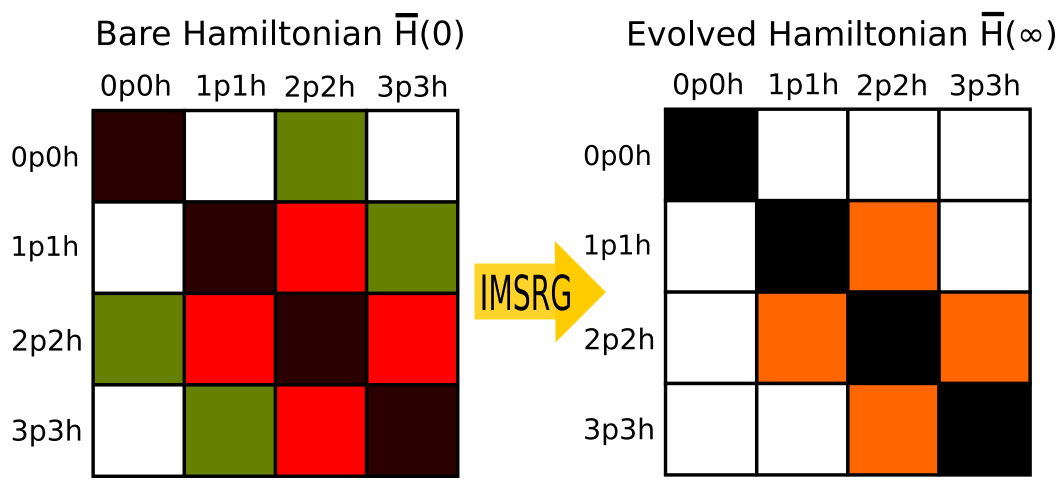
In-medium similarity renormalization group (IM-SRG)

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

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

$$s = 0 \rightarrow \infty$$

Figure from Nathan Parzuchowski



K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011).

In-medium similarity renormalization group (IM-SRG)

- Evolve Hamiltonian via flow equation: $\frac{d\widetilde{H}}{ds} = \left[\eta(s), \widetilde{H}(s)\right]$

  where $\eta(s) \equiv \frac{dU}{ds} U^{\dagger}(s) = [G, \widetilde{H}(s)]$ is the IM-SRG generator
- Choose G to specify type of flow

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

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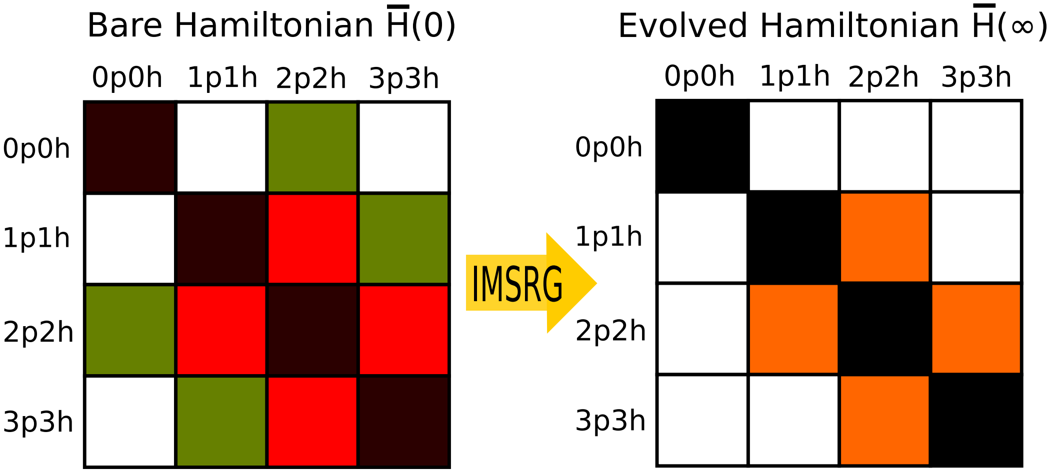

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The Magnus Expansion: Formalism

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

$$\frac{d\Omega}{ds} = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega}^{k}(\eta) = \eta - \frac{1}{2}[\Omega, \eta] + \frac{1}{12}[\Omega, [\Omega, \eta]] + \cdots$$

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

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- Evolved Hamiltonian (or any operator) given by $\mathrm{H}(s) = e^{\Omega} H e^{-\Omega}$
- Converges to IM-SRG result as $k \to \infty$
- Successive terms fall off by $\frac{1}{k!}$

  $\rightarrow$ Sum is truncated for practical calculations

The Magnus Expansion: Motivation

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  - Eigenvalues of evolved operator are preserved
  - No need for high-order ODE solver – use first-order Euler method

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  - No loss in accuracy in observables despite crude method

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- Modest computational speed-up and substantial memory savings when solving for several operators

For more details, see T.D. Morris, N.M. Parzuchowski, S.K. Bogner, Phys. Rev. C **92**, 034331 (2015)

Test Case for the Magnus expansion

1. Within the IM-SRG, intruder states (low-lying states in valence space) can distort the evolved Hamiltonian
   - This is not well understood for IM-SRG transformations
   - Does the choice of generator affect this?

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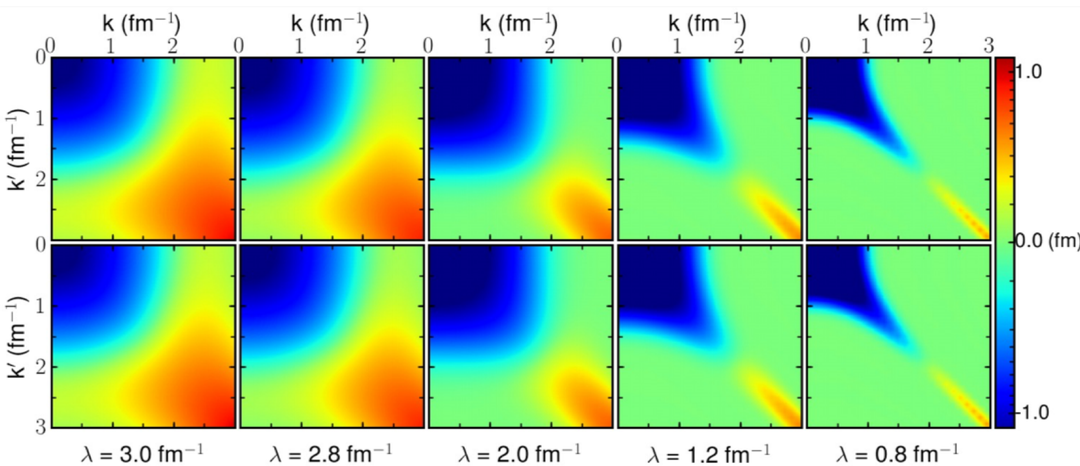
- Due to the use of the Magnus expansion in IM-SRG, we must also answer the following:

2. Does the Magnus expansion converge to the typical IM-SRG for these types of problems?
   - Before addressing 1, we must understand 2
   - Here we apply the Magnus expansion in free-space using an analogous problem as a test case*

*Note: the Magnus expansion holds for SRG as well as IM-SRG

SRG formalism



SRG evolution of $V_\lambda(k, k')$ for several values of $\lambda = s^{-1/4}$

$G = T_{rel}$ (relative kinetic energy)

$G = \widetilde{H}_d(s)$ (diagonal of $\widetilde{H}(s)$, "Wegner")

- SRG softens Hamiltonian by decoupling low- and high-momenta
- For typical chiral NN potentials, same $\widetilde{H}(s)$ regardless of $\mathrm{G} = T_{rel}$ or $\widetilde{H}_d(s)$!

Figure from K.A. Wendt, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **83**, 034005 (2011)

Test Case: NN potentials with large χEFT cutoffs

- Typical cutoff sizes for χEFT in nuclear structure: $\Lambda{\sim}500\ MeV$
- Nogga, Timmermans, and van Kolck* took Λ to much higher values to study cutoff dependence in chiral nuclear interactions
- Here we consider $\Lambda = 4.0, 9.0\ fm^{-1} \approx 800, 1800\ MeV$ at LO with non-local regulator

*A. Nogga, R.G.E. Timmermans, and U. van Kolck, Phys. Rev. C **72**, 054006 (2005)

Test Case: NN potentials with large χEFT cutoffs

- $\Lambda = 4.0, 9.0\ fm^{-1} \approx 800, 1800\ MeV$ at LO
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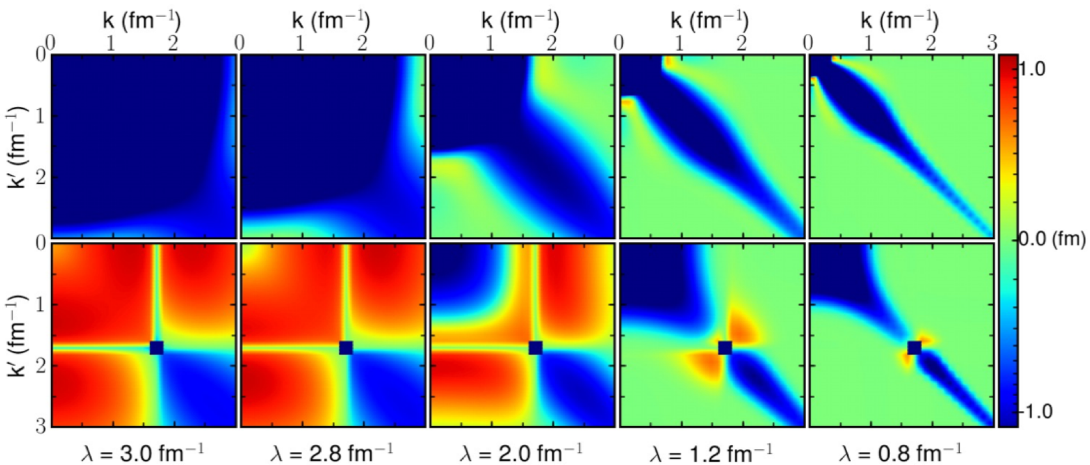
  - From EFT perspective, deeply bound states are outside of range of EFT
  - In practice, do they corrupt low-momentum physics?
- The SRG has shown sensitivity to choice of G for these potentials: how does the Magnus expansion respond to large χEFT cutoffs?

Test Case: NN potentials with large χEFT cutoffs



SRG evolution of $V_\lambda(k, k')$ with $\Lambda = 9.0\ fm^{-1}$ for several values of λ

$G = T_{rel}$ (relative kinetic energy)

$G = \widetilde{H}_d(s)$ (diagonal of $\widetilde{H}(s)$, "Wegner")

- Wendt, Furnstahl, and Perry demonstrated SRG evolution of these potentials with T_{rel} and Wegner generators
  - T_{rel} : spurious bound state distorts the low-momentum block of $H(s)$ (analogous to intruder states in IM-SRG)
  - Wegner: keeps spurious bound state safely outside low-momentum block

Figure from K.A. Wendt, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **83**, 034005 (2011)

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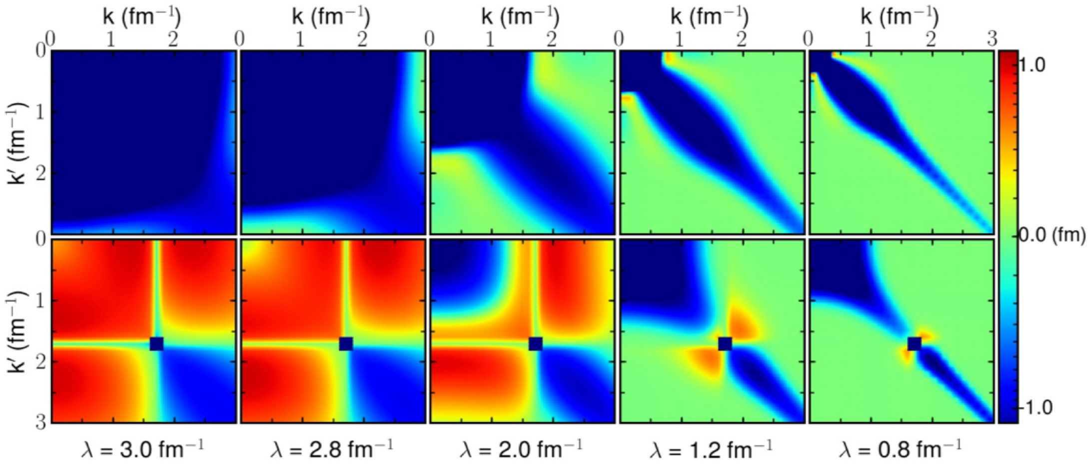

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- Wendt, Furnstahl, and Perry demonstrated SRG evolution of these potentials with T_{rel} and Wegner generators
  - E.g., deuteron wave function at low-momentum is significantly affected by the spurious bound state with T_{rel} but not with Wegner
  - Choice in G matters unlike case before!
  - Good test problem for the Magnus expansion

Figure from K.A. Wendt, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **83**, 034005 (2011)

Results: Magnus v. typical SRG

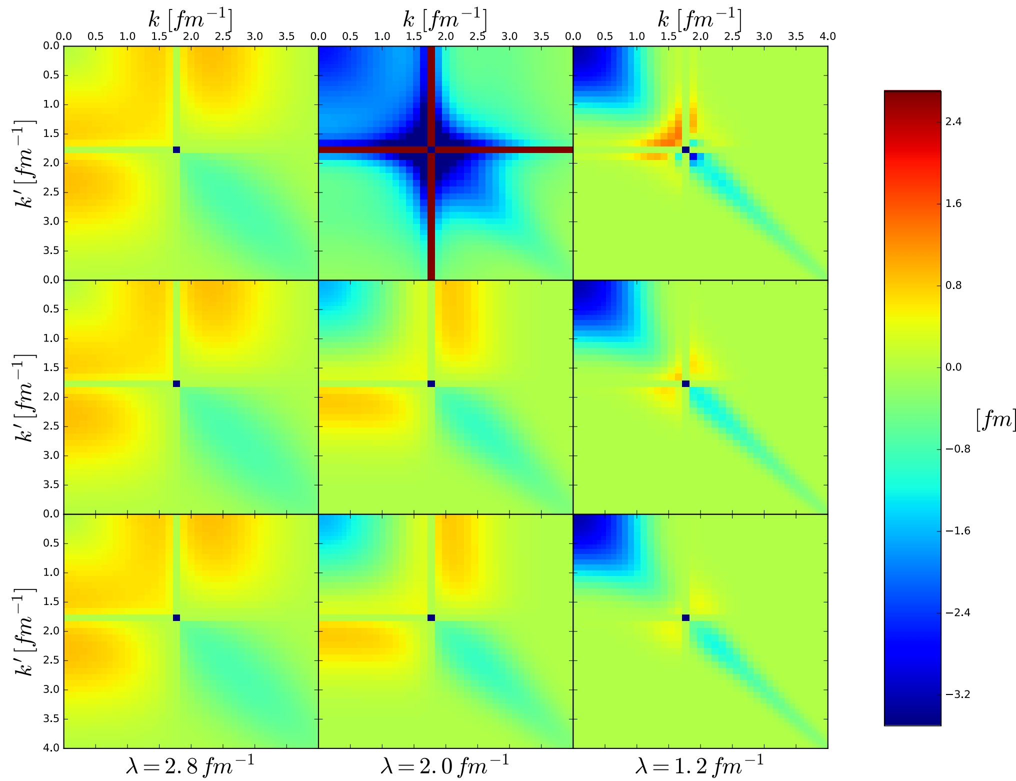
- Low-truncation in Magnus expansion gives undesirable results
- Magnus converges to SRG around $k \sim 4$
- Spurious deeply bound state does not distort low-momentum block with Wegner generator

Contours of $V_\lambda(k, k')$ with $\Lambda = 9.0\ fm^{-1}$ and $\mathrm{G} = \widetilde{H}_d(s)$ for several values of λ

Magnus, $k = 2$

Magnus, $k = 4$

SRG



Results: Magnus v. typical SRG

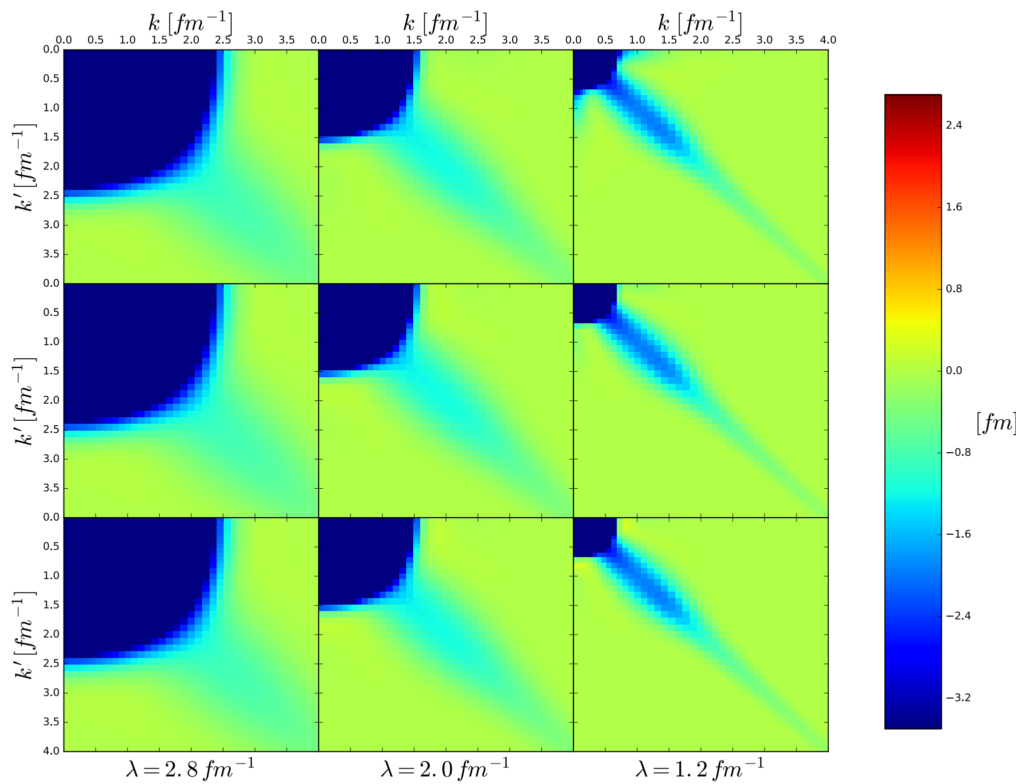
- Spurious bound state shifted to low-momentum
- The evolution of spurious bound states matches the SRG result regardless of truncation on the Magnus expansion

Contours of $V_\lambda(k, k')$ with $\Lambda = 9.0\ fm^{-1}$ and $\mathrm{G} = T_{rel}$ for several values of λ

Magnus, $k = 2$

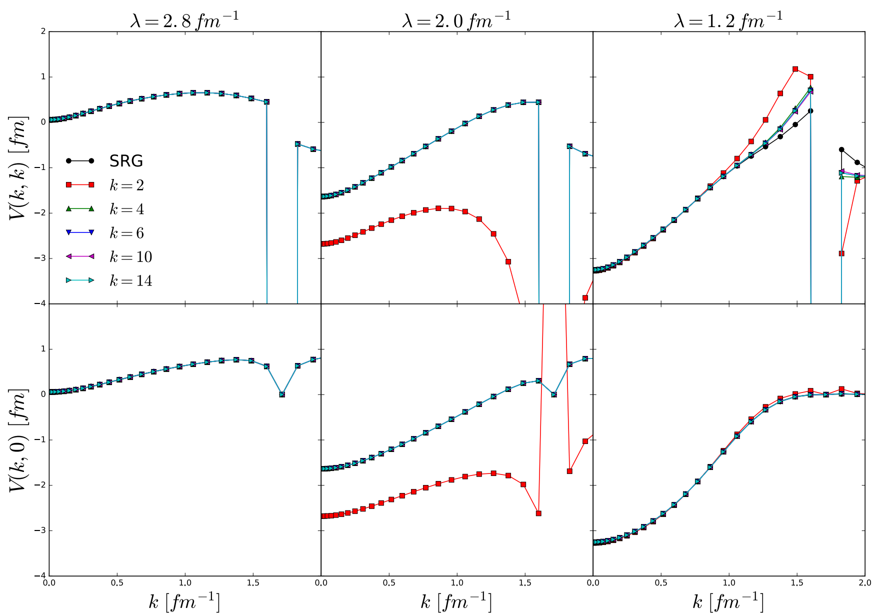
Magnus, $k = 4$

SRG

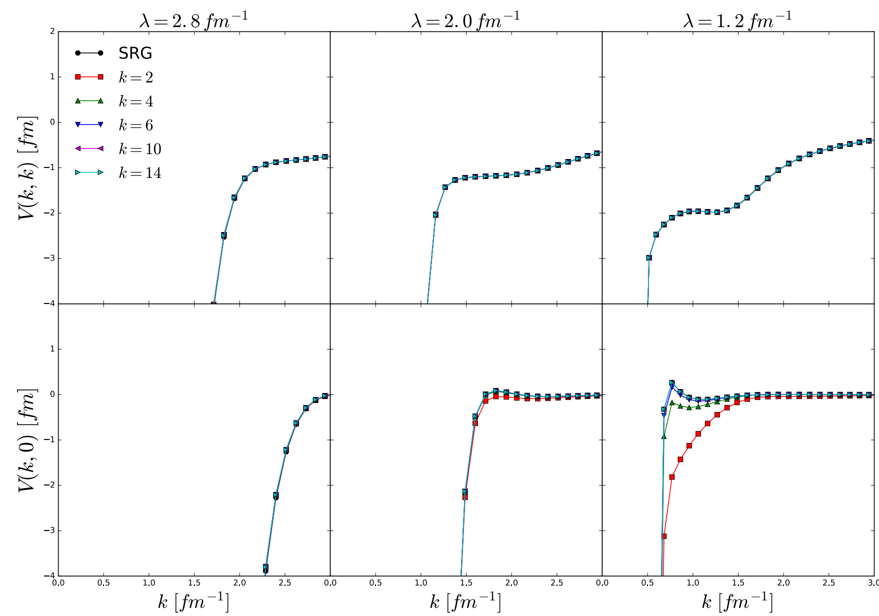


Results: Magnus v. typical SRG

- At sufficiently high truncations in the series ($k \gtrsim 4$), Magnus implementation matches SRG ($\Lambda = 9.0\ fm^{-1}$ in figure)



$\mathrm{G} = \widetilde{H}_d(s)$



$\mathrm{G} = T_{rel}$

Results: Accuracy of observables

- $U(s)$ is a unitary transformation and should preserve observables
- Relative error of deuteron binding energy:

$$\delta\varepsilon_d = \left|\frac{\varepsilon_d - \widetilde{\varepsilon_d}}{\varepsilon_d}\right|$$

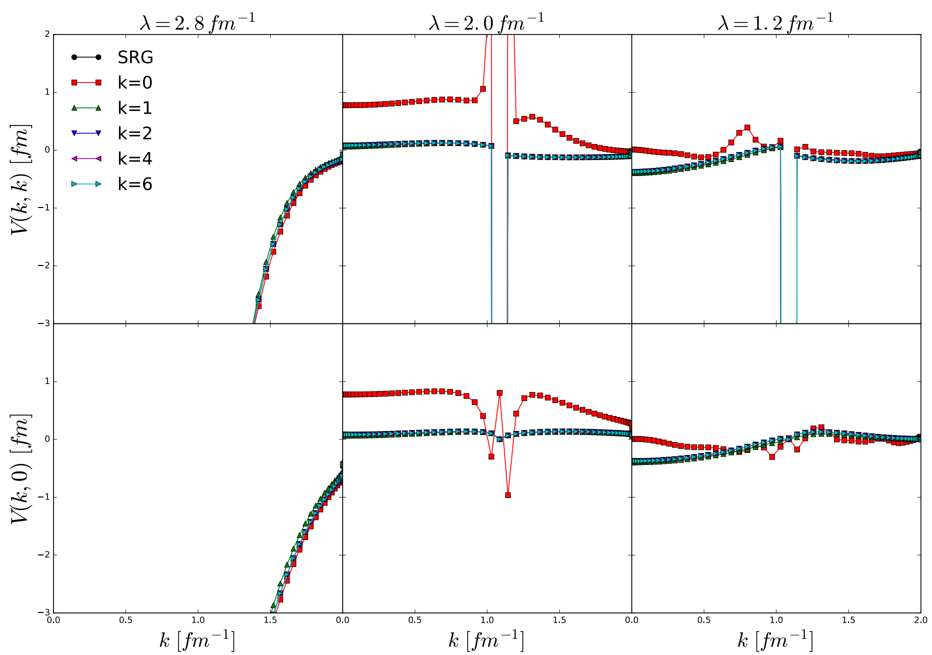
where $\widetilde{\varepsilon_d}$ corresponds to the evolved Hamiltonian

SRG: $\delta\varepsilon_d \sim 10^{-6}$ (compounds error in solving ODE)

Magnus: $\delta\varepsilon_d \sim 10^{-13}$

Results: Non- v. semi-local potentials

- Previous results were with non-local regulator
- Consider LO semi-local potential
  - Non-local regulator for contact force
  - Local regulator for pion exchange
- Magnus matches SRG evolution at lower k for semi-local potential



$G = \widetilde{H}_d(s)$ and $\Lambda = 4.0\ fm^{-1}$

Results: Non- v. semi-local potentials

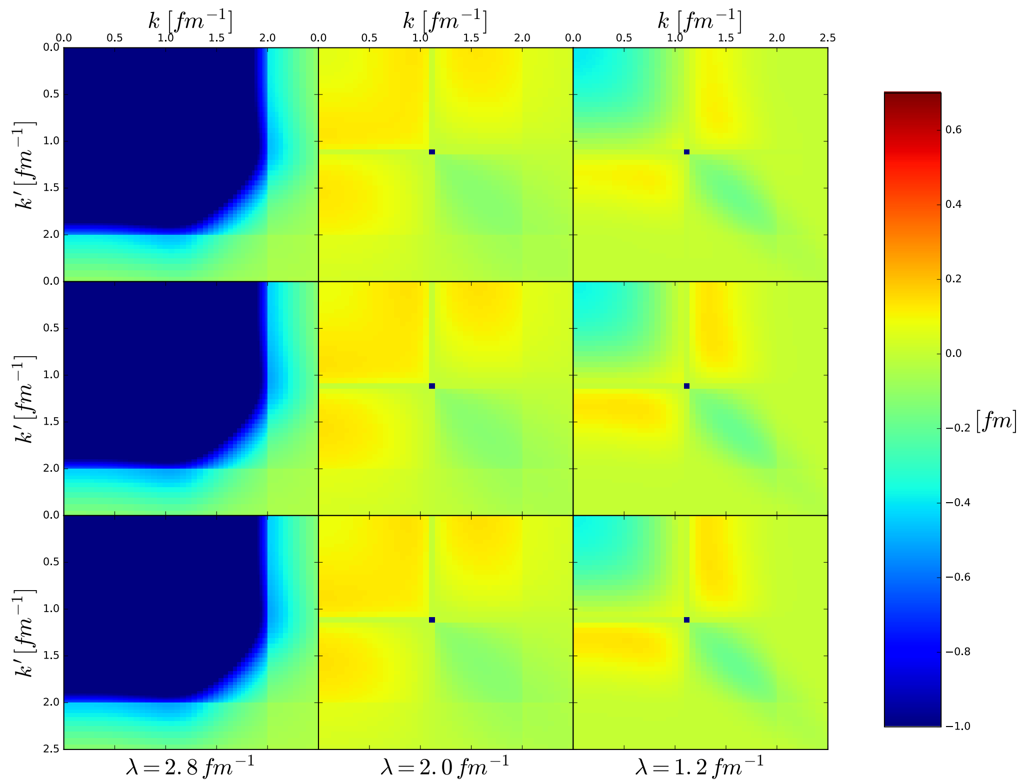
- Spurious deeply bound state appears at $\Lambda = 4.0\ fm^{-1}$ in semi-local potential
- Dependence on Λ changes from the details of the regulator (i.e., form of non-local/local)

Contours of semi-local $V_\lambda(k, k')$ with $\Lambda = 4.0\ fm^{-1}$ and $\mathrm{G} = \widetilde{H}_d(s)$ for several values of λ

Magnus, $k = 1$

Magnus, $k = 2$

SRG



Summary

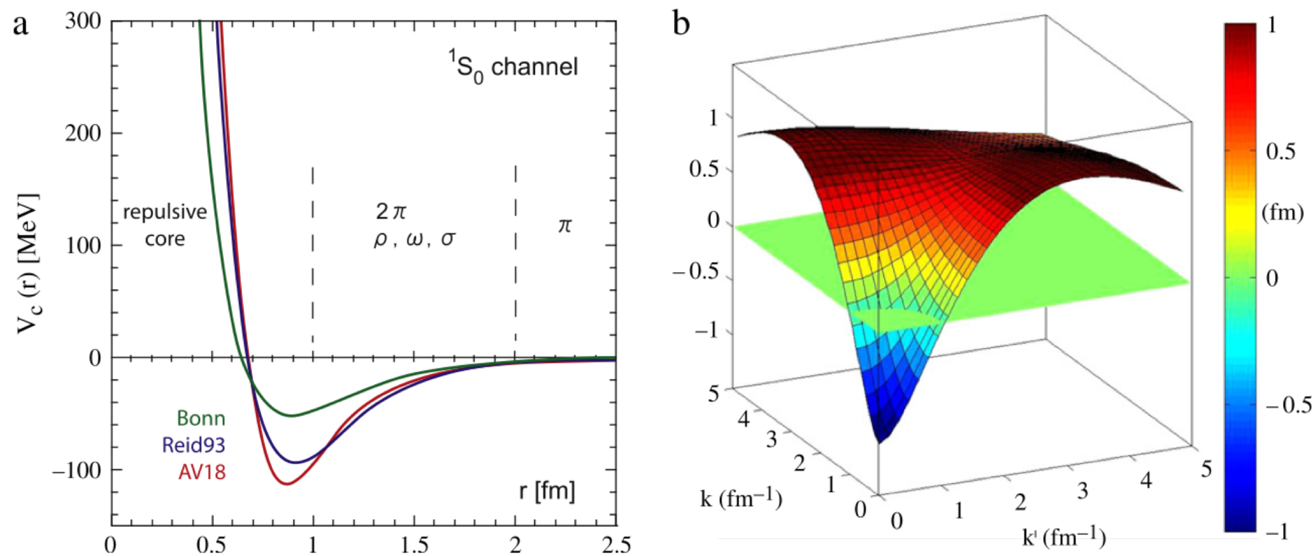
- Magnus expansion improves viability/efficiency of the SRG
- SRG evolution sensitive to generator at high Λ
- Magnus implementation matches SRG Wegner and T_{rel} evolution (given high enough truncation)
- Magnus implementation converges to SRG result at even lower truncations for semi-local potential

Outlook

- IM-SRG with the Magnus expansion
  - Does the sensitivity to choice of generator carry over to Magnus/IM-SRG nuclear structure calculations?
- High Λ and regulator*
  - How does the placement of spurious bound state depend on Λ and regulator?
  - How can Λ be compared for different regulators?

*Renewed interest on this problem! Upcoming paper by Tews, Huth, and Schwenk tests local chiral potentials at high cutoffs.

Back-up slides



Several phenomenological NN potentials (left) and momentum-space matrix elements of AV18 (right)

Figure from S.K. Bogner, R.J. Furnstahl, and A. Schwenk, Prog. Part. Nucl. Phys. **65**, 94 (2010)