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

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NUCLEI

Nuclear Computational Low-Energy Initiative

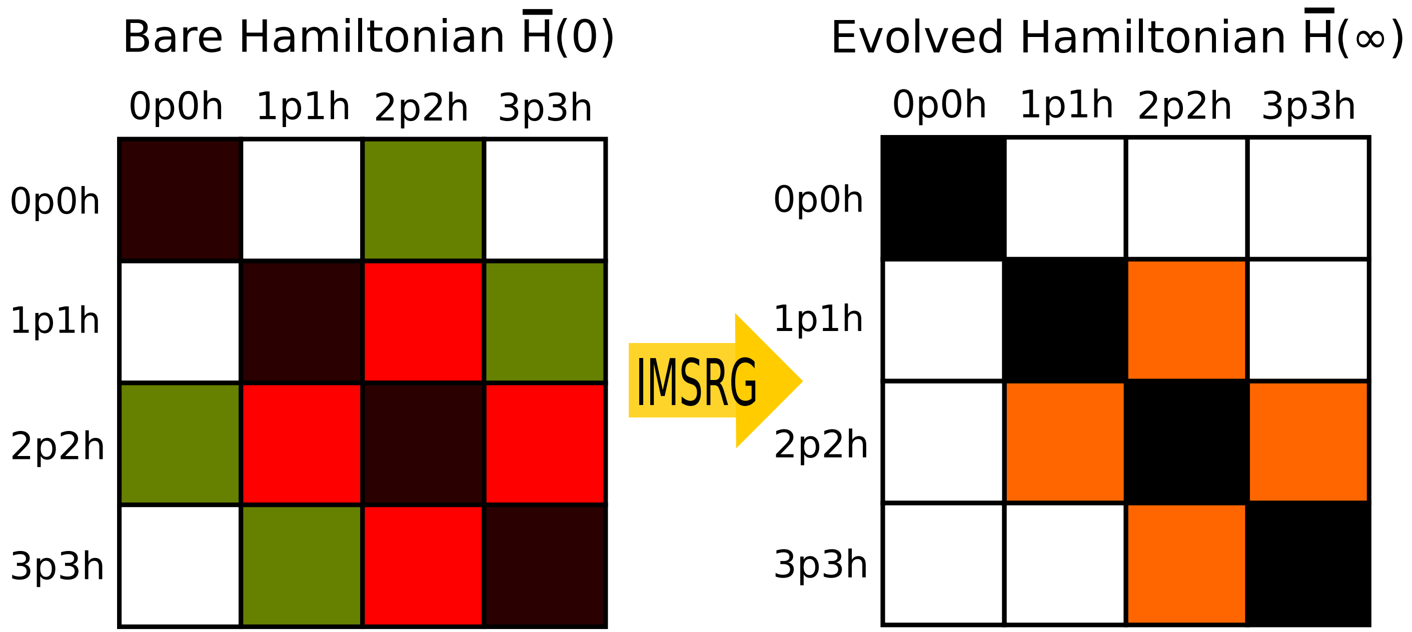
In-medium similarity renormalization group (IM-SRG)

- Free-space SRG decouples low- and high-momenta to simplify operators
- IM-SRG solves the many-body problem by decoupling the reference state from particle/hole excitations

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

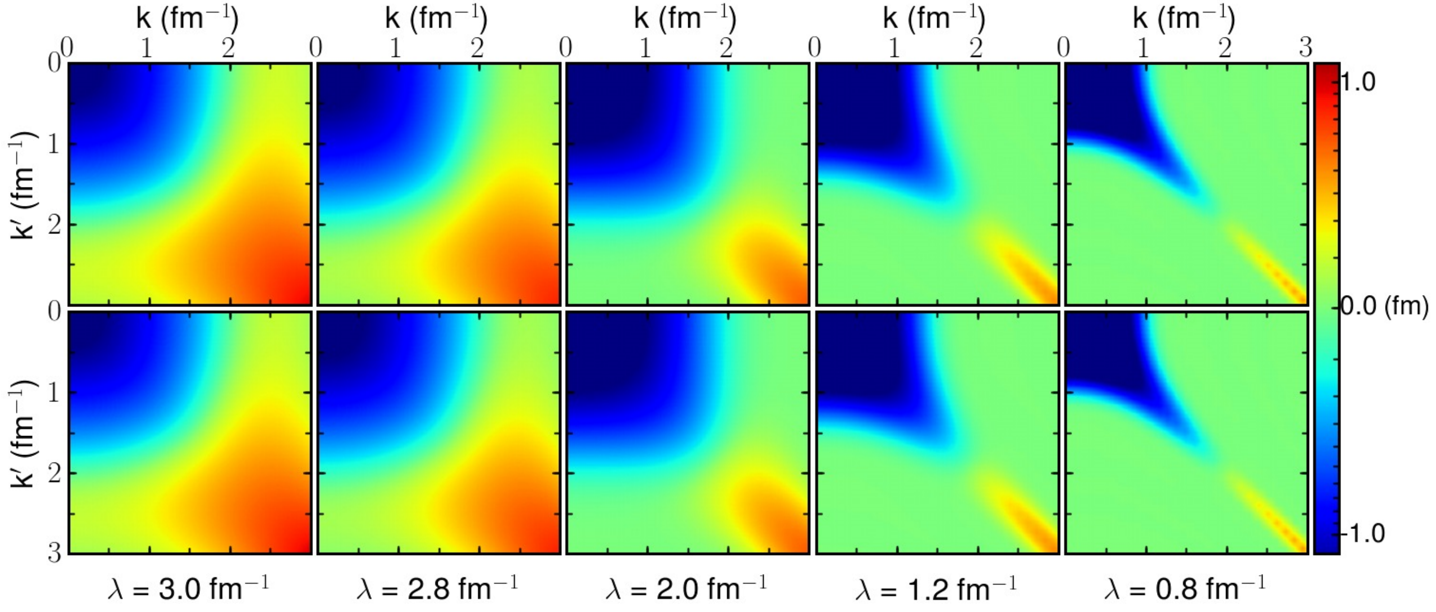
$$s = 0 \ \rightarrow \ \infty$$

Figure from Nathan Parzuchowski



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

SRG formalism



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

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

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

- Primary interest is the application of the Magnus expansion to the IM-SRG, but here we use free-space SRG to test the Magnus expansion
- Evolve Hamiltonian via flow equation: $\frac{d\widetilde{H}}{ds} = \left[\eta(s), \widetilde{H}(s)\right]$

  where $\eta(s) = [G, \widetilde{H}(s)]$ is the SRG generator

- 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)

The Magnus Expansion: Formalism

- Solution of the form $U(s) = e^{\Omega(s)}$ exists
- Solve for $\Omega(s)$ 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

- Converges to SRG result as $k \to \infty$
- Successive terms fall off by $\frac{1}{k!}$

  → Sum is truncated for practical calculations

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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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- 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: 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

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

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    - At short distances (high momenta), the Hamiltonian is highly singular featuring spurious deeply bound states (which are non-physical) due to short-range tensor forces
    - Does not corrupt low-energy physics so long as spurious bound states are at sufficiently high momentum
- The SRG has shown sensitivity to choice of G for these potentials: how does the Magnus expansion respond to large χEFT cutoffs?

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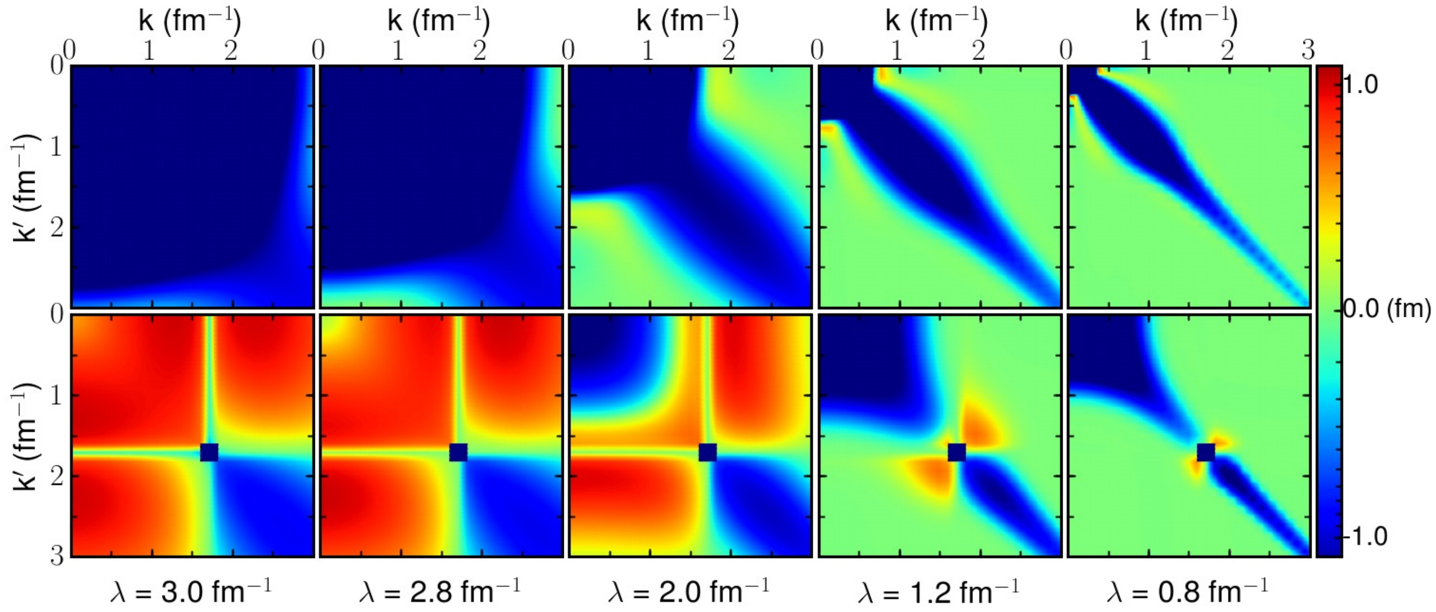
Test Case: NN potentials with large χEFT cutoffs cont…



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

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

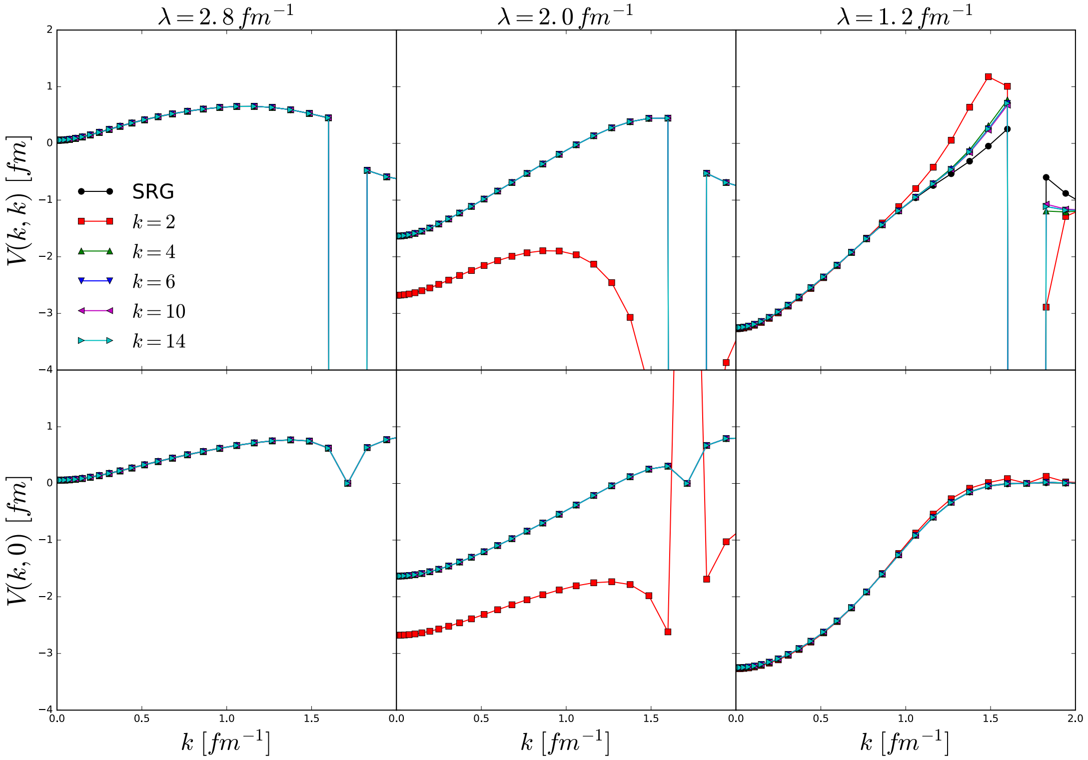
$\mathrm{G} = \widetilde{H}_d(s)$ (diagonal of $\widetilde{H}(s)$, “Wegner“)

- 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
  - Choice in G matters unlike case before!
  - Good test problem for the Magnus expansion

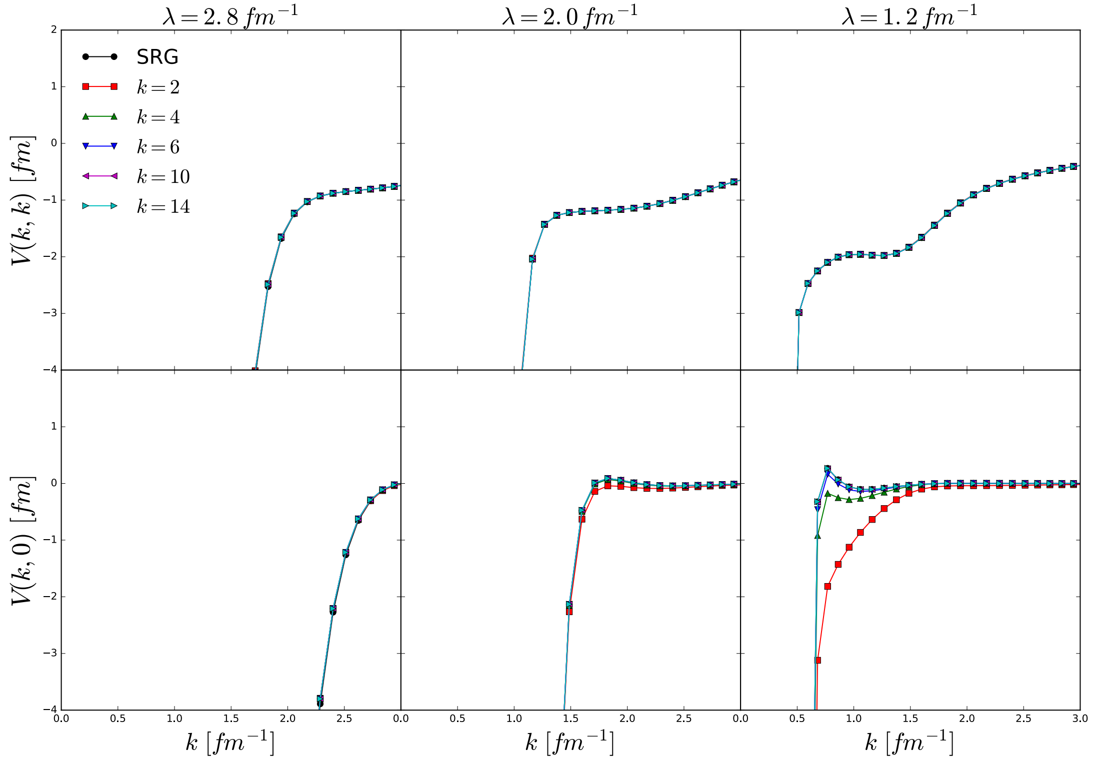
Figure from [*]K.A. Wendt, R.J. Furnstahl, R.J. Perry, Phys. Rev. C **83**, 034005 (2011)

Results: Magnus v. typical SRG

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



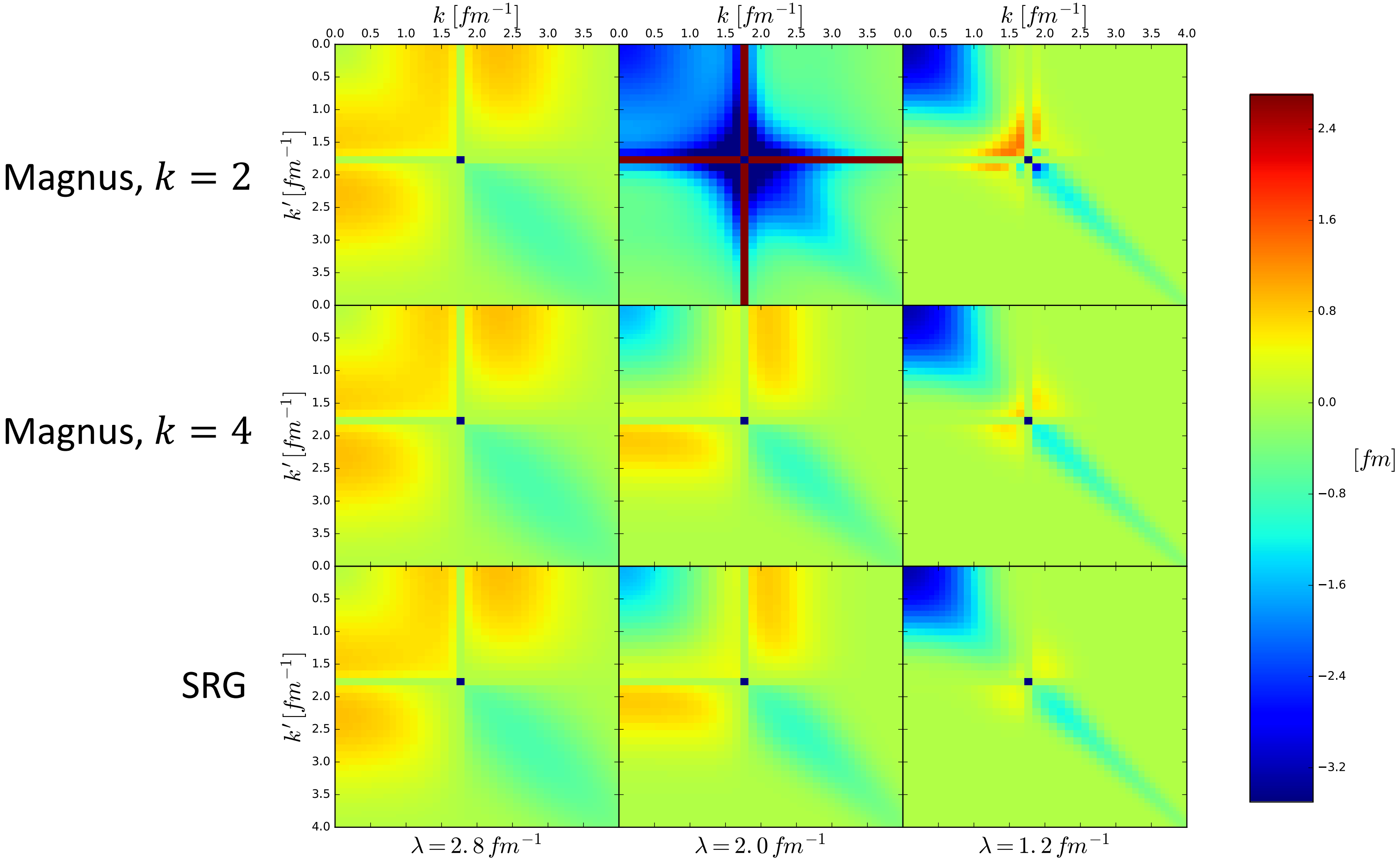
$\mathrm{G} = \widetilde{H}_d(s)$



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

Results: Truncation of series

- 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

Results: Accuracy of 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

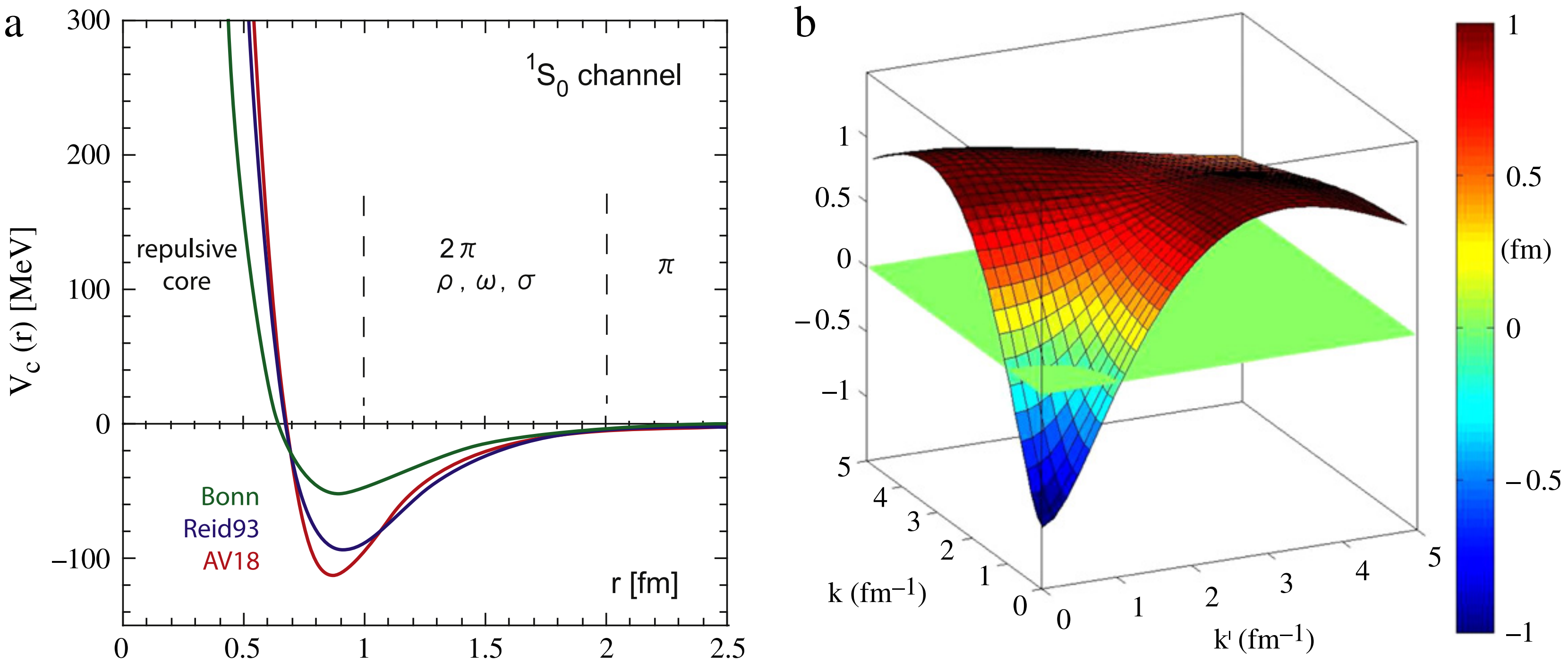
SRG: $\delta\varepsilon_d \sim 10^{-6}$ (compounds error in solving ODE)

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

Summary and outlook

- Magnus expansion improves viability/efficiency of the SRG
- Magnus implementation matches SRG Wegner and T_{rel} generator evolution (given high enough truncation)
- Does the sensitivity to choice of generator carry over to IM-SRG nuclear structure calculations?
- How does the Magnus evolve non- v. semi-local potentials?

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)