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Block diagonalization using similarity renormalization group flow equations

E. Anderson,[1] S. K. Bogner,[2] R. J. Furnstahl,[1] E. D. Jurgenson,[1] R. J. Perry,[1] and A. Schwenk[3]
[1]*Department of Physics, The Ohio State University, Columbus, Ohio 43210, USA*
[2]*National Superconducting Cyclotron Laboratory and*
Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48844, USA
[3]*TRIUMF, 4004 Wesbrook Mall, Vancouver, British Columbia, Canada V6T 2A3*
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By choosing appropriate generators for the Similarity Renormalization Group (SRG) flow equations, different patterns of decoupling in a Hamiltonian can be achieved. Sharp and smooth block-diagonal forms of phase-shift equivalent nucleon-nucleon potentials in momentum space are generated as examples and compared to analogous low-momentum interactions ("$V_{\text{low}\,k}$").

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The Similarity Renormalization Group (SRG) [1–3] applied to internucleon interactions is a continuous series of unitary transformations implemented as a flow equation for the evolving Hamiltonian H_s,

$$\frac{dH_s}{ds} = [\eta_s, H_s] = [[G_s, H_s], H_s]. \tag{1}$$

Here s is a flow parameter and the flow operator G_s specifies the type of SRG [4]. Decoupling between low-energy and high-energy matrix elements is naturally achieved in a momentum basis by choosing a momentum-diagonal flow operator such as the kinetic energy T_{rel} or the diagonal of H_s; either drives the Hamiltonian toward *band-diagonal* form. This decoupling leads to dramatically improved variational convergence in few-body nuclear systems compared to unevolved phenomenological or chiral effective field theory (EFT) potentials [5,6].

Renormalization Group (RG) methods that evolve NN interactions with a sharp or smooth cutoff in relative momentum, known generically as $V_{\text{low}\,k}$, rely on the invariance of the two-nucleon T matrix [7,8]. These approaches achieve a *block-diagonal* form characterized by a cutoff Λ (see left plots in Figs. 1 and 2). As implemented in Refs. [7,8], the high-momentum matrix elements are defined to be zero, but this is not required.

Block-diagonal decoupling of the sharp $V_{\text{low}\,k}$ form can be generated using SRG flow equations by choosing a block-diagonal flow operator (see Refs. [9,10] for details),

$$G_s = \begin{pmatrix} PH_sP & 0 \\ 0 & QH_sQ \end{pmatrix} \equiv H_s^{\text{bd}}, \tag{2}$$

with projection operators P and $Q = 1 - P$. In a partial-wave momentum representation, P and Q are step functions defined by a sharp cutoff Λ on relative momenta. This choice for G_s, which means that η_s is nonzero only where G_s is zero, suppresses off-diagonal matrix elements such that the Hamiltonian approaches a block-diagonal form as s increases. If one considers a measure of the off-diagonal coupling of the Hamiltonian,

$$\text{Tr}\,[(QH_sP)^\dagger(QH_sP)] = \text{Tr}\,[PH_sQH_sP] \geqslant 0, \tag{3}$$

then its derivative is easily evaluated by applying the SRG equation, Eq. (1):

$$\begin{aligned}\frac{d}{ds}&\text{Tr}\,[PH_sQH_sP]\\ &= \text{Tr}\,[P\eta_sQ(QH_sQH_sP - QH_sPH_sP)]\\ &\quad + \text{Tr}\,[(PH_sPH_sQ - PH_sQH_sQ)Q\eta_sP]\\ &= -2\,\text{Tr}\,[(Q\eta_sP)^\dagger(Q\eta_sP)] \leqslant 0.\end{aligned} \tag{4}$$

Thus, the off-diagonal QH_sP block will decrease in general as s increases [9,10].

The right plots in Figs. 1 and 2 result from evolving the N^{3}LO potential from Ref. [11] using the block-diagonal G_s of Eq. (2) with $\Lambda = 2\,\text{fm}^{-1}$ until $\lambda \equiv 1/s^{1/4} = 0.5\,\text{fm}^{-1}$. The parameter λ is a quantitative measure of the progress toward block diagonalization made by the SRG evolution. The agreement between $V_{\text{low}\,k}$ and SRG potentials for momenta below Λ is striking. A similar degree of universality is found in the other partial waves. Deriving an explicit connection between these approaches is the topic of an ongoing investigation.

The evolution with λ of two representative partial waves ($^3\text{S}_1$ and $^1\text{P}_1$) are shown in Figs. 3 and 4. The evolution of the "off-diagonal" matrix elements (meaning those outside the PH_sP and QH_sQ blocks) can be roughly understood from the dominance of the kinetic energy on the diagonal. Let the indices p and q run over indices of the momentum states in the P and Q spaces, respectively. To good approximation we can replace PH_sP and QH_sQ by their eigenvalues E_p and E_q in the SRG equations, yielding [9,10]

$$\frac{d}{ds}h_{pq} \approx \eta_{pq}E_q - E_p\eta_{pq} = -(E_p - E_q)\eta_{pq} \tag{5}$$

and

$$\eta_{pq} \approx E_ph_{pq} - h_{pq}E_q = (E_p - E_q)h_{pq}. \tag{6}$$

Combining these two results, we have the evolution of any off-diagonal matrix element:

$$\frac{d}{ds}h_{pq} \approx -(E_p - E_q)^2h_{pq}. \tag{7}$$

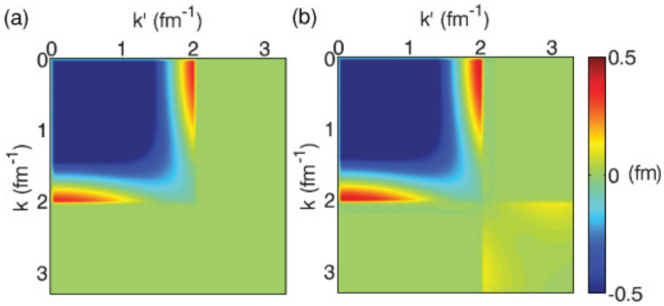

FIG. 1. (Color online) Comparison of momentum-space (a) $V_{\mathrm{low}\,k}$ and (b) SRG block-diagonal potentials with $\Lambda = 2\,\mathrm{fm}^{-1}$ evolved from an N^{3}LO $^3S_1$ potential [11].

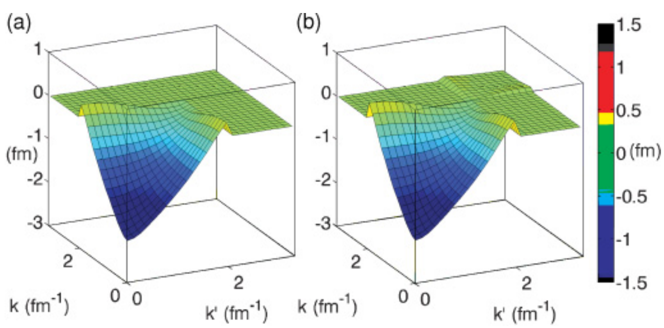

FIG. 2. (Color online) Comparison of momentum-space (a) $V_{\mathrm{low}\,k}$ and (b) SRG block-diagonal potentials with $\Lambda = 2\,\mathrm{fm}^{-1}$ evolved from an N^{3}LO $^3S_1$ potential [11].

In the NN case we can replace the eigenvalues by those for the relative kinetic energy, giving an explicit solution

$$h_{pq}(s) \approx h_{pq}(0)e^{-s(\epsilon_p-\epsilon_q)^2} \tag{8}$$

with $\epsilon_p \equiv p^2/M$. Thus the off-diagonal elements go to zero with the energy differences just like with the SRG with T_{rel}; one can see the width of order $1/\sqrt{s} = \lambda^2$ in the k^2 plots of the evolving potential in Figs. 3 and 4.

While in principle the evolution to a sharp block-diagonal form means going to $s = \infty(\lambda = 0)$, in practice we need only take s as large as needed to quantitatively achieve the decoupling implied by Eq. (8). Furthermore, it should hold for more general definitions of P and Q. To smooth out the cutoff, we can introduce a smooth regulator f_Λ, which we take here to be an exponential form:

$$f_\Lambda(k) = e^{-(k^2/\Lambda^2)^n}, \tag{9}$$

with n an integer. For $V_{\mathrm{low}\,k}$ potentials, typical values used are $n = 4$ and $n = 8$ (the latter is considerably sharper but still numerically robust). By replacing H_s^{bd} with

$$G_s = f_\Lambda H_s f_\Lambda + (1 - f_\Lambda)H_s(1 - f_\Lambda), \tag{10}$$

we get a smooth block-diagonal potential.

A representative example with $\Lambda = 2\,\mathrm{fm}^{-1}$ and $n = 4$ is shown in Fig. 5. We can evolve to $\lambda = 1.5\,\mathrm{fm}^{-1}$ without a problem. For smaller λ the overlap of the P and Q spaces becomes significant and the potential becomes distorted. This distortion indicates that there is no further benefit to evolving

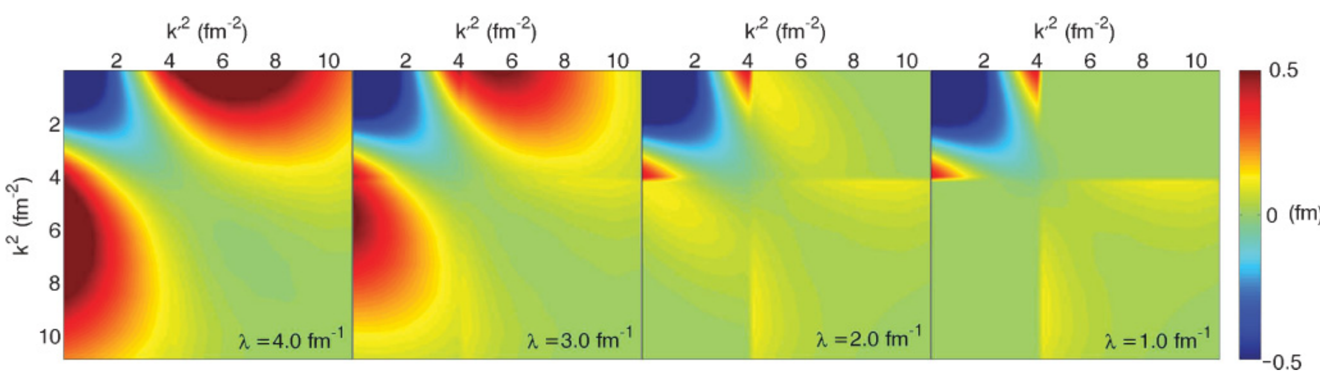

FIG. 3. (Color online) Evolution of the $^3S_1$ partial wave with a sharp block-diagonal flow equation with $\Lambda = 2\,\mathrm{fm}^{-1}$ at $\lambda = 4, 3, 2$, and $1\,\mathrm{fm}^{-1}$. The initial N^{3}LO potential is from Ref. [11].

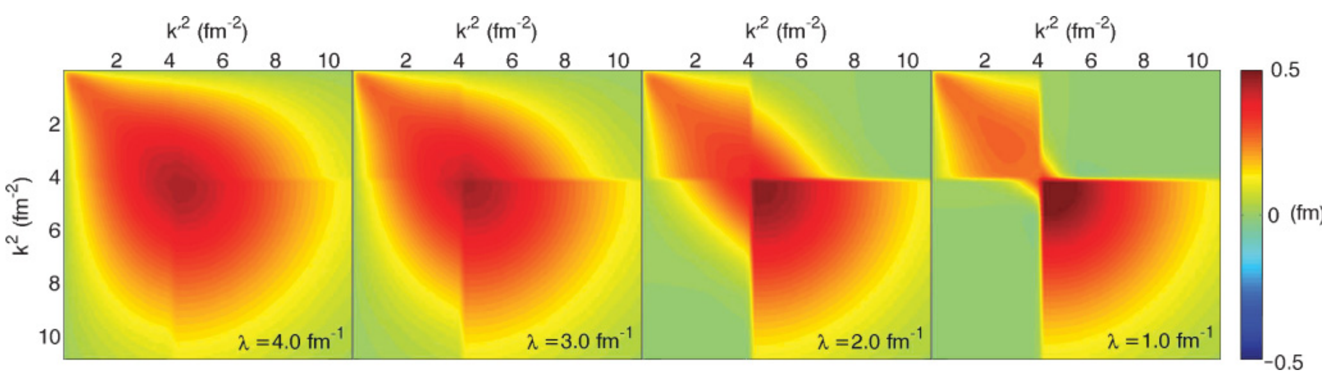

FIG. 4. (Color online) Same as Fig. 3 but for the $^1P_1$ partial wave.

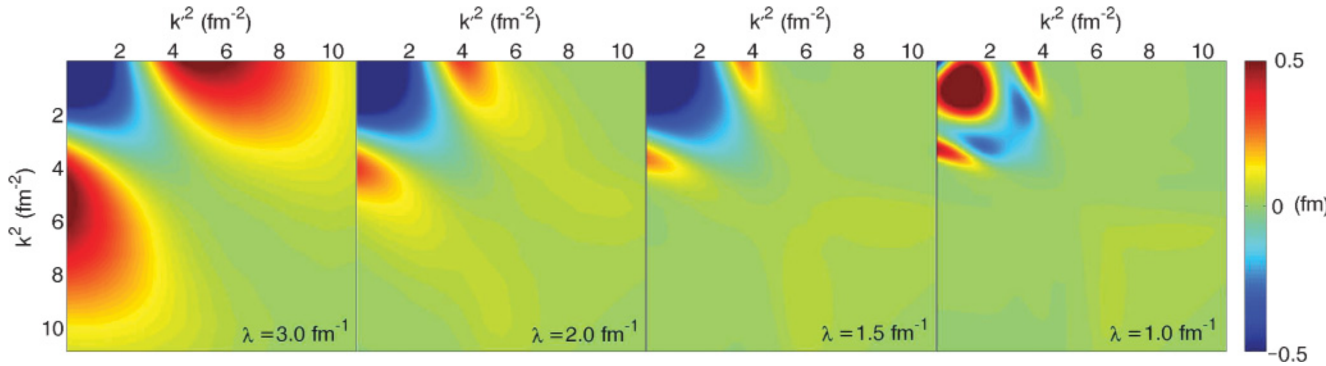

FIG. 5. (Color online) Evolution of the $^3S_1$ partial wave with a smooth ($n = 4$) block-diagonal flow equation with $\Lambda = 2.0\,\mathrm{fm}^{-1}$, starting with the N^{3}LO potential from Ref. [11]. The flow parameter λ is 3, 2, 1.5, and 1 fm^{-1}.

in λ very far below Λ; in fact the decoupling worsens for $\lambda < \Lambda$ with a smooth regulator.

Another type of SRG that is second-order exact and yields similar block diagonalization is defined by

$$\eta_s = [T, PV_sQ + QV_sP], \tag{11}$$

which can be implemented with $P \to f_\Lambda$ and $Q \to (1 - f_\Lambda)$, with f_Λ either sharp or smooth. We can also consider bizarre choices for f_Λ in Eq. (10), such as defining it to be zero out to Λ_{lower}, then unity out to Λ, and then zero above that. This means that $1 - f_\Lambda$ defines both low and high-momentum blocks and the region that is driven to zero consists of several rectangles. Results for two partial waves starting from the Argonne v_{18} potential [12] are shown in Fig. 6. Despite

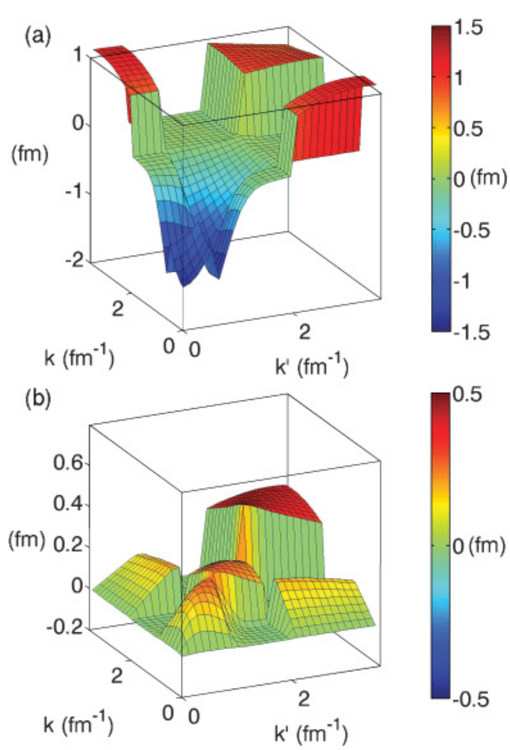

FIG. 6. (Color online) Evolved SRG potentials starting from Argonne v_{18} in the (a) $^1S_0$ and (b) $^1P_1$ partial waves to $\lambda = 1\,\mathrm{fm}^{-1}$ using a bizarre choice for G_s (see text).

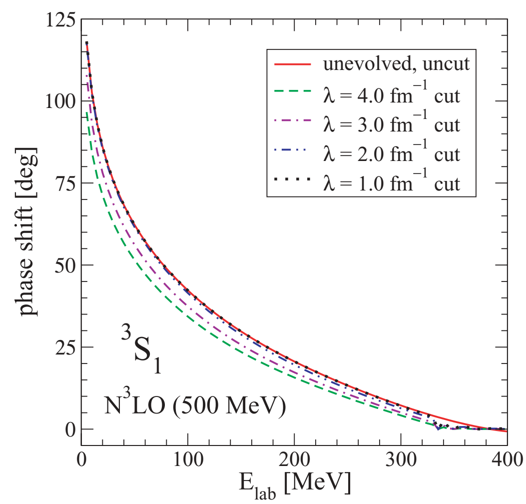

FIG. 7. (Color online) Phase shifts for the $^3S_1$ partial wave from an initial N^{3}LO potential and the evolved sharp SRG block-diagonal potential with $\Lambda = 2\,\mathrm{fm}^{-1}$ at various λ, in each case with the potential set identically to zero above Λ.

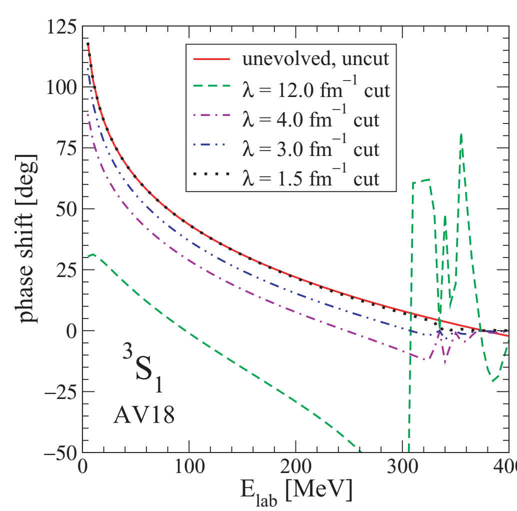

FIG. 8. (Color online) Same as Fig. 7 but with Argonne v_{18} as the initial potential [12].

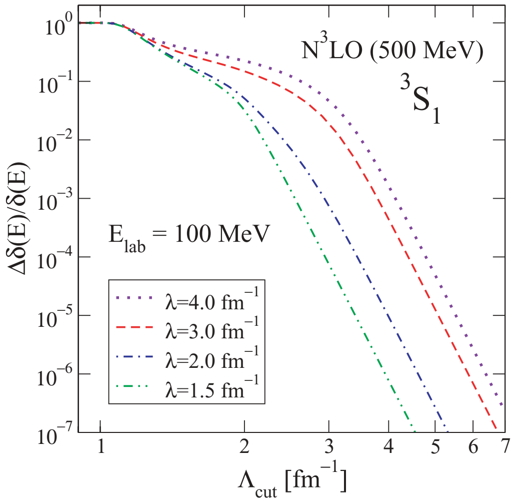

FIG. 9. (Color online) Errors in the phase shift at $E_{\rm lab} = 100$ MeV for the evolved sharp SRG block-diagonal potential with $\Lambda = 2\,\text{fm}^{-1}$ for a range of λ's and a regulator with $n = 8$.

the strange appearance, these remain unitary transformations of the original potential, with phase shifts and other NN observables the same as with the original potential. These choices provide a proof-of-principle that the decoupled regions can be tailored to the physics problem at hand.

Definitive tests of decoupling for NN observables are now possible for $V_{\text{low}\,k}$ potentials since the unitary transformation of the SRG guarantees that no physics is lost. For example, in Figs. 7 and 8 we show $^3S_1$ phase shifts from an SRG sharp block diagonalization with $\Lambda = 2\,\text{fm}^{-1}$ for two different potentials. The phase shifts are calculated with the potentials cut sharply at Λ. That is, the matrix elements of the potential are set to zero above that point. The improved decoupling as λ decreases is evident in each case. By $\lambda = 1\,\text{fm}^{-1}$ in Fig. 7, the unevolved and evolved curves are indistinguishable to the width of the line up to about 300 MeV.

In Fig. 9 we show a quantitative analysis of the decoupling as in Ref. [13]. The figure shows the relative error of the phase shift at 100 MeV calculated with a potential that is cut off by a smooth regulator as in Eq. (9) at a series of values $\Lambda_{\rm cut}$. We observe the same universal decoupling behavior seen in Ref. [13]: a shoulder indicating the perturbative decoupling region, where the slope matches the power $2n$ fixed by the smooth regulator. The onset of the shoulder in $\Lambda_{\rm cut}$ decreases with λ until it saturates for λ somewhat below Λ, leaving the shoulder at $\Lambda_{\rm cut} \approx \Lambda$. Thus, as $\lambda \to 0$ the decoupling scale is set by the cutoff Λ.

In the more conventional SRG, where we use $\eta_s = [T, H_s] = [T, V_s]$, it is easy to see that the evolution of the two-body potential in the two-particle system can be carried over directly to the three-particle system. In particular, it follows that the three-body potential does not depend on disconnected two-body parts [4,14]. If we could implement η_s as proposed here with analogous properties, we would have a tractable method for generating $V_{\text{low}\,k}$ three-body forces. While it seems possible to define Fock-space operators with projectors P and Q that will not have problems with disconnected parts, it is not yet clear whether full decoupling in the few-body space can be realized. Work on this problem is in progress.

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