LLNL-JRNL-412933

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May 11, 2009

Physical Review Letters

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Evolution of Nuclear Many-Body Forces with the Similarity Renormalization Group

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The first practical method to evolve many-body nuclear forces to softened form using the Similarity Renormalization Group (SRG) in a harmonic oscillator basis is demonstrated. When applied to ^{4}He calculations, the two- and three-body oscillator matrix elements yield rapid convergence of the ground-state energy with a small net contribution of the induced four-body force.

PACS numbers: 21.30.-x,05.10.Cc,13.75.Cs

A major goal of nuclear structure theory is to make quantitative calculations of low-energy nuclear observables starting from microscopic internucleon forces. Chiral effective field theory (χEFT) provides a systematic construction of these forces, including a hierarchy of many-body forces of decreasing strength [1]. Renormalization group (RG) methods can be used to soften the short-range repulsion and short-range tensor components of the initial chiral interactions so that convergence of nuclear structure calculations is greatly accelerated [2, 3]. The difficulty is that these transformations (or any other softening transformations) change the short-range many-body forces. To account for these changes, we present in this letter the first consistent evolution of three-body forces by using the Similarity Renormalization Group (SRG) [4–8], which offers a technically simpler approach to evolving many-body forces than other RG formulations. Our results show that both the many-body hierarchy of χEFT and the improved convergence properties are preserved.

The SRG is a series of unitary transformations of the free-space Hamiltonian ($H \equiv H_{\lambda=\infty}$),

$$H_\lambda = U_\lambda H_{\lambda=\infty} U_\lambda^\dagger \,, \tag{1}$$

labeled by a momentum parameter λ that runs from ∞ toward zero,[1] which keeps track of the sequence of Hamiltonians. These transformations are implemented as a flow equation in λ,

$$\frac{dH_\lambda}{d\lambda} = -\frac{4}{\lambda^5}[[T, H_\lambda], H_\lambda] \,, \tag{2}$$

whose form guarantees that the H_λ's are unitarily equivalent [6, 7].

The appearance of the nucleon kinetic energy T in Eq. (2) leads to high- and low-momentum parts of H_λ being decoupled, which means softer and more convergent potentials [9]. This is evident in a partial-wave momentum basis, where matrix elements $\langle k|H_\lambda|k'\rangle$ connecting states with (kinetic) energies differing by more than λ^2 are suppressed by $e^{-(k^2-k'^2)^2/\lambda^4}$ factors and therefore the states decouple as λ decreases. (Decoupling also results from replacing T in Eq. (2) with other generators [6, 7, 10].) The optimal range for λ is not yet established and also depends on the system, but experience with SRG and other low-momentum potentials suggest that running to about $\lambda = 2.0\,\mathrm{fm}^{-1}$ (in units where $\hbar^2/M = 1$) is a good compromise between improved convergence from decoupling and the growth of induced many-body interactions [9].

To see how the two-, three-, and higher-body potentials are identified, it is useful to decompose H_λ in second-quantized form. Schematically (suppressing indices and sums),

$$H_\lambda = \langle T\rangle a^\dagger a + \langle V_\lambda^{(2)}\rangle a^\dagger a^\dagger a a + \langle V_\lambda^{(3)}\rangle a^\dagger a^\dagger a^\dagger a a a + \cdots \,, \tag{3}$$

where $a^\dagger$, a are creation and destruction operators with respect to the vacuum in some (coupled) single-particle basis. This *defines* $\langle V_\lambda^{(2)}\rangle$, $\langle V_\lambda^{(3)}\rangle$, ... as the two-body, three-body, ... matrix elements at each λ. Upon evaluating the commutators in Eq. (2) using H_λ from Eq. (3), we find that even if initially there are only two-body potentials, higher-body potentials are generated with each step in λ. Thus, when applied in an A-body subspace, the SRG will "induce" A-body forces. But we also find that $\langle T\rangle$ is fixed, $\langle V_\lambda^{(2)}\rangle$ is determined entirely in the $A = 2$ subspace with no dependence on $\langle V_\lambda^{(3)}\rangle$, $\langle V_\lambda^{(3)}\rangle$ is determined in $A = 3$ given $\langle V_\lambda^{(2)}\rangle$, and so on.

Since only the Hamiltonian enters the SRG evolution equations, there are no difficulties with solving T matrices in all channels for different A-body systems. However, in a momentum basis there will be complications from disconnected terms associated with spectator nucleons, which require solving separate equations for each set of $\langle V_\lambda^{(n)}\rangle$ matrix elements. In Refs. [11, 12], a diagrammatic approach is introduced to handle these complications. But while it is natural to solve Eq. (2) in momentum representation, we can in fact use any convenient basis. Having chosen a basis, we obtain coupled first-order differential equations for the matrix elements of the flowing Hamiltonian H_λ, where the right side of Eq. (2) is evaluated using simple matrix multiplications.

[1] The flow parameter $s = 1/\lambda^4$ has been used for the SRG elsewhere [7, 8].

Here we choose to evolve in a *discrete* basis, where there are no issues with disconnected terms and induced many-body forces can be directly identified.

Our calculations are performed in the Jacobi coordinate harmonic oscillator (HO) basis of the No-Core Shell Model (NCSM) [13]. This is a translationally invariant, anti-symmetric basis for each A, with a complete set of states up to a maximum excitation of $N_{\rm max}\hbar\Omega$ above the minimum energy configuration, where Ω is the harmonic oscillator parameter. The procedures used here build directly on Ref. [12], which presents a one-dimensional implementation of our approach along with a general analysis of the evolving many-body hierarchy.

We start by evolving H_λ in the $A=2$ subsystem, which completely fixes the two-body matrix elements $\langle V_\lambda^{(2)}\rangle$. Next, by evolving H_λ in the $A=3$ subsystem we determine the combined two-plus-three-body matrix elements. We can isolate the three-body matrix elements by subtracting the evolved $\langle V_\lambda^{(2)}\rangle$ elements in the $A=3$ basis [12]. Having obtained the separate NN and NNN matrix elements, we can apply them to any nucleus. We are also free to include any initial three-nucleon force in the initial Hamiltonian without changing the procedure. If applied to $A\geq 4$, four-body (and higher) forces will not be included and so the transformations will be only approximately unitary. The questions to be addressed are whether the decreasing hierarchy of many-body forces is maintained and whether the induced four-body contribution is unnaturally large. We summarize in Table I the different calculations to be made for ^{3}H and ^{4}He to confront these questions.

The initial ($\lambda=\infty$) NN potential used here is the 500 MeV N^{3}LO interaction from Ref. [14]. The initial NNN potential is the N^{2}LO interaction [15] in the local form of Ref. [16] with constants fit to the average of triton and ^{3}He binding energies and triton beta decay according to Ref. [17]. We expect similar results from other initial interactions because the SRG drives them toward near universal form; a survey will be given in Ref. [18]. NCSM calculations with these initial interactions and the parameter set in Table I of Ref. [17] yield energies of $-8.473(4)$ MeV for ^{3}H and $-28.50(2)$ MeV for ^{4}He compared with -8.482 MeV and -28.296 MeV from experiment, respectively. So there is a 20 keV uncertainty in the calculation of ^{4}He from incomplete convergence and a 200 keV discrepancy with experiment. The latter is consistent with the omission of three- and four-body chiral interactions at N^{3}LO. These provide a scale for assessing whether induced four-body contributions are important compared to other uncertainties.

In Fig. 1, the ground-state energy of the triton is plotted as a function of the flow parameter λ. Evolution is from $\lambda=\infty$, which is the initial (or "bare") interaction, toward $\lambda=0$. We use $N_{\rm max}=36$ and $\hbar\Omega=28$ MeV, for which all energies are converged to better than 10 keV. We first consider an NN interaction with no initial NNN ("NN-only"). If H_λ is evolved only in an $A=2$ system, higher-body induced pieces are lost. The resulting energy calculations will only be approximately unitary for $A>2$ and the ground-state energy will vary with λ (squares). Keeping the induced NNN yields a flat line (circles), which implies an exactly unitary transformation; the line is equally flat if an initial NNN is included (diamonds). Note that the net induced three-body is comparable to the initial NNN contribution and thus is of natural size.

In Fig. 2, we examine the SRG evolution in λ for ^{4}He with $\hbar\Omega=36$ MeV. The $\langle V_\lambda^{(2)}\rangle$ and $\langle V_\lambda^{(3)}\rangle$ matrix elements were evolved in $A=2$ and $A=3$ with $N_{\rm max}=28$

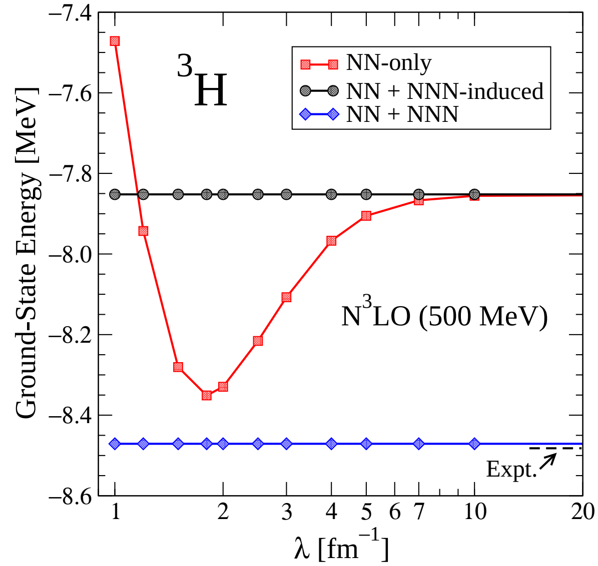

FIG. 1: (Color online) Ground-state energy of ^{3}H as a function of the SRG evolution parameter, λ. See Table I for the nomenclature of the curves.

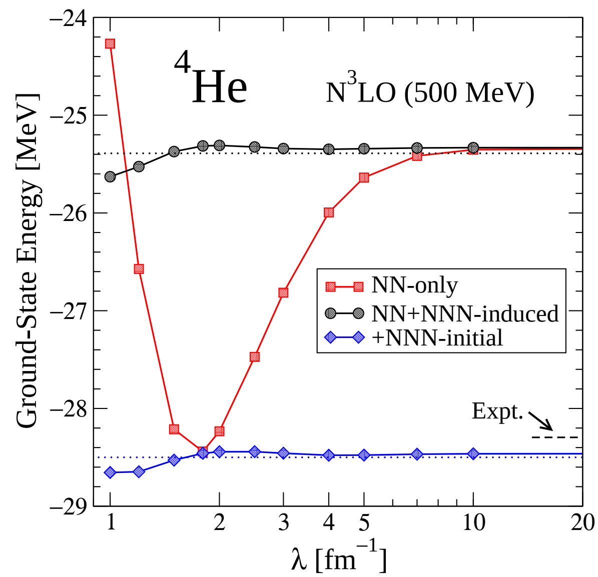

FIG. 2: (Color online) Ground-state energy of ^{4}He as a function of the SRG evolution parameter, λ. See Table I for the nomenclature of the curves.

TABLE I: Definitions of the various calculations.

NN-only	No initial NNN interaction and do not keep NNN-induced interaction.
NN + NNN-induced	No initial NNN interaction but keep the SRG-induced NNN interaction.
NN + NNN	Include an initial NNN interaction *and* keep the SRG-induced NNN interaction.

and then truncated to $N_{\max} = 18$ at each λ to diagonalize ^{4}He. The NN-only curve has a similar shape as for the triton. In fact, this pattern of variation has been observed in all SRG calculations of light nuclei [3]. When the induced NNN is included, the evolution is close to unitary and the pattern only depends slightly on an initial NNN interaction. In both cases the dotted line represents the converged value for the initial Hamiltonian. At large λ, the discrepancy is due to a lack of convergence at $N_{\max} = 18$, but at $\lambda < 3\,\mathrm{fm}^{-1}$ SRG decoupling takes over and the discrepancy is due to induced four-body forces, which therefore contribute about 50 keV net at $\lambda = 2\,\mathrm{fm}^{-1}$. This is small compared to the rough estimate in Ref. [19] that the contribution from the long-ranged part of the N^{3}LO four-nucleon force to ^{4}He binding is of order a few hundred keV. If needed, we could evolve 4-body matrix elements in $A = 4$ and will do so when nuclear structure codes can accomodate them.

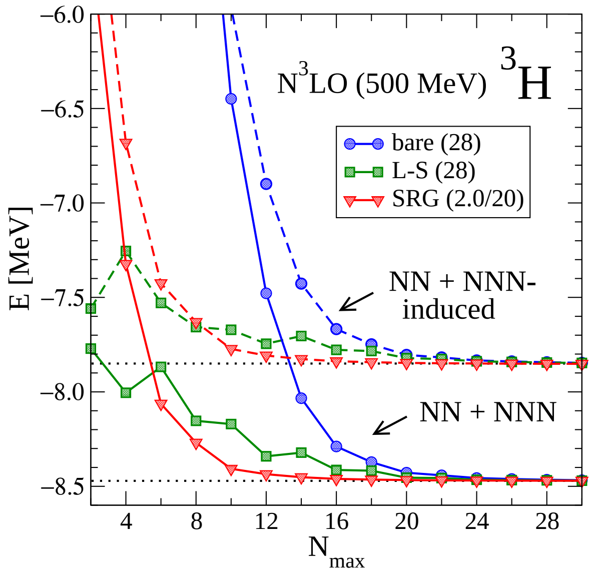

FIG. 3: (Color online) Ground-state energy of ^{3}H as a function of the basis size $N_{\max}$ for an N^{3}LO NN interaction [14] with and without an initial NNN interaction [1, 17]. Unevolved ("bare") and Lee-Suzuki (L-S) results with $\hbar\Omega = 28$ MeV are compared with SRG at $\hbar\Omega = 20$ MeV evolved to $\lambda = 2.0\,\mathrm{fm}^{-1}$.

In Fig. 3, we show the triton ground-state energy as a function of the oscillator basis size, $N_{\max}$, for various calculations. The lower (upper) curves are with (without) an initial three-body force (see Table I). The convergence of the bare interaction is compared with the SRG evolved to $\lambda = 2.0\,\mathrm{fm}^{-1}$. The oscillator parameter $\hbar\Omega$ in each case was chosen roughly to optimize the convergence of each Hamiltonian. (As λ decreases, so does the optimal $\hbar\Omega$.) We also compare to a Lee-Suzuki (L-S) effective interaction, which has been used in the NCSM to greatly improve convergence [20, 21]. These effective interactions result from unitary transformations within the model space of a given nucleus, in contrast to the free-space transformation of the SRG.

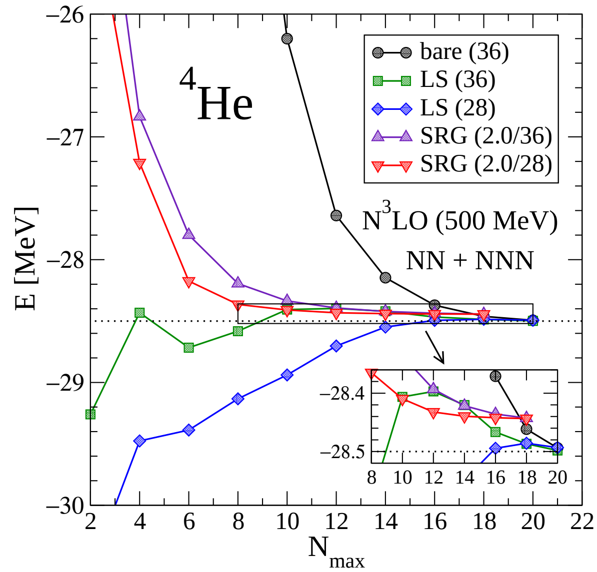

FIG. 4: (Color online) Ground-state energy of ^{4}He as a function of the basis size $N_{\max}$ for an N^{3}LO NN interaction [14] with an initial NNN interaction [1, 17]. Unevolved (bare) results are compared with Lee-Suzuki (L-S) and SRG evolved to $\lambda = 2.0\,\mathrm{fm}^{-1}$ at $\hbar\Omega = 28$ and 36 MeV.

The SRG calculations are variational and converge smoothly and rapidly from above with or without an initial three-body force. The dramatic improvement in convergence rate is seen even though the χEFT interaction is relatively soft. Thus, once evolved, a much smaller $N_{\max}$ basis is adequate for a desired accuracy and extrapolating in $N_{\max}$ is also feasible.

Figure 4 illustrates for ^{4}He the same rapid convergence with $N_{\max}$ of an SRG-evolved interaction. However, in this case the asymptotic value of the energy differs slightly because of the omitted induced four-body contribution. (The SRG-evolved asymptotic values for different $\hbar\Omega$ differ by only 10 keV, so the gap between the converged bare/L-S results and the SRG results is dominated by the induced NNNN rather than incomplete convergence). Convergence is even faster for lower λ values [18], ensuring a useful range for the analysis of few-

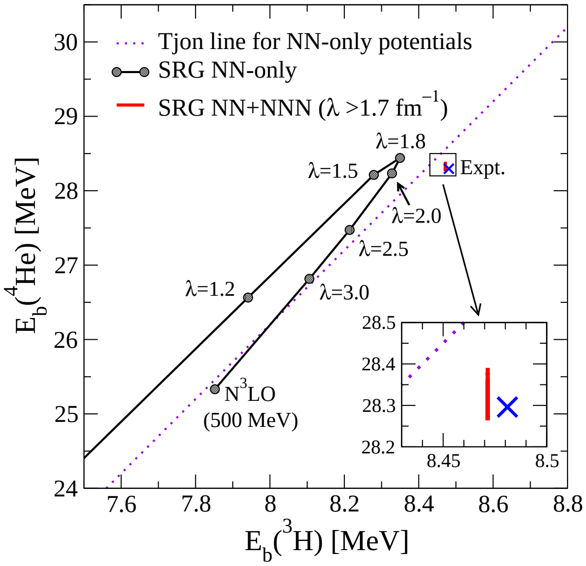

FIG. 5: (Color online) Binding energy of the alpha particle vs. the binding energy of the triton. The Tjon line from phenomenological NN potentials (dotted) is compared with the trajectory of SRG energies when only the NN interaction is kept (circles). When the initial and induced NNN interactions are included, the trajectory lies close to experiment for $\lambda > 1.7\,\mathrm{fm}^{-1}$ (see inset).

body systems. However, because of the strong density dependence of four-nucleon forces, it will be important to monitor the size of the induced four-body contributions for heavier nuclei and nuclear matter.

The impact of evolving the full three-body force is neatly illustrated in Fig. 5, where the binding energy of ^{4}He is plotted against the binding energy of ^{3}H. The experimental values of these quantities, which are known to a small fraction of a keV, define only a point in this plane (at the center of the X, see inset). The SRG NN-only results trace out a trajectory in the plane that is analogous to the well-known Tjon line (dotted), which is the approximate locus of points for phenomenological potentials fit to NN data but not including NNN [22]. In contrast, the short trajectory of the SRG with the NN + NNN interaction (shown for $\lambda \geq 1.8\,\mathrm{fm}^{-1}$) highlights the small variations from the omitted four-nucleon force. Note that a trajectory plotted for NN+NNN-induced calculations would be a similarly small line at the N^{3}LO NN-only point.

In summary, we have demonstrated a practical method to use the SRG to evolve NNN (and higher many-body) forces in a harmonic oscillator basis. Calculations of $A \leq 4$ nuclei including NNN show the same favorable convergence properties observed elsewhere for NN-only, with a net induced four-body contribution in $A = 4$ that is smaller than the truncation errors of the chiral interaction. The soft SRG interactions are an alternative to the use of Lee-Suzuki effective interactions in NCSM and the HO matrix elements can also be used (after conversion to a Slater-determinant HO basis as needed) for coupled cluster and many-body perturbation theory calculations. A more complete analysis of convergence and dependencies for the energy and other observables for few-body systems, as well as results for other interactions and choices of generator in Eq. (2), will be given in a forthcoming publication [18].

Acknowledgments

We thank E. Anderson, S. Bogner, J. Drut, R. Perry, S. Quaglioni, and A. Schwenk for useful comments. This work was supported in part by the National Science Foundation under Grant No. PHY–0653312 and the UNEDF SciDAC Collaboration under DOE Grant DE-FC02-07ER41457. Prepared in part by LLNL under Contract DE-AC52-07NA27344.

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