In-Medium Similarity Renormalization Group For Nuclei

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We present a new *ab initio* method that uses similarity renormalization group (SRG) techniques to continuously diagonalize nuclear many-body Hamiltonians. In contrast with applications of the SRG to two- and three-nucleon interactions in free space, we perform the SRG evolution "in medium" directly in the A-body system of interest. The in-medium approach has the advantage that one can approximately evolve $3, \ldots, A$-body operators using only two-body machinery based on normal-ordering techniques. The method is nonperturbative and can be tailored to problems ranging from the diagonalization of closed-shell nuclei to the construction of effective valence-shell Hamiltonians and operators. We present first results for the energies of ^{4}He, ^{16}O, and ^{40}Ca, which have accuracies comparable to coupled-cluster calculations.

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Great progress has been made in *ab initio* nuclear structure over the past decade, where it is now possible to calculate properties of light nuclei up to about carbon [1,2] and low-lying states of medium-mass nuclei near closed shells [3,4]. A key challenge in nuclear physics is to extend this *ab initio* frontier to larger and open-shell systems. This requires methods that can handle the strong coupling between low and high momenta in nuclear forces used in these calculations.

In recent years, new approaches to nuclear forces based on renormalization group (RG) ideas have been developed that decouple high-momentum degrees of freedom by lowering the resolution (or a cutoff) scale in nuclear forces to typical nuclear structure momentum scales [5]. Such RG-evolved potentials, known generically as "low-momentum interactions," greatly simplify the nuclear many-body problem and enhance the convergence of structure and reaction calculations, while the freedom to vary the resolution scale provides a powerful tool to assess theoretical uncertainties due to truncations in the Hamiltonian and from many-body approximations [5–8].

One path to decouple high-momentum degrees of freedom is the similarity renormalization group (SRG), which was introduced independently by Glazek and Wilson [9] and Wegner [10]. The SRG consists of a continuous sequence of unitary transformations that suppress off-diagonal matrix elements, driving the Hamiltonian towards a band- or block-diagonal form. Writing the unitarily transformed Hamiltonian as

$$H(s) = U(s)HU^\dagger(s) \equiv H^d(s) + H^{od}(s), \tag{1}$$

where $H^d(s)$ and $H^{od}(s)$ are the appropriately defined "diagonal" and "off-diagonal" parts of the Hamiltonian, the evolution with the flow parameter s is given by

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

Here $\eta(s) \equiv [dU(s)/ds]U^\dagger(s)$ is the anti-Hermitian generator of the transformation. The choice of the generator first suggested by Wegner,

$$\eta(s) = [H^d(s), H(s)] = [H^d(s), H^{od}(s)], \tag{3}$$

guarantees that the off-diagonal coupling of H^{od} is driven exponentially to zero with increasing s [10]. Through different choices for H^d and H^{od}, one can tailor the SRG evolution to transform the initial Hamiltonian to a form that is most convenient for a particular problem [11,12]. It is this flexibility, together with the fact that one never explicitly constructs and applies the unitary transformation $U(s)$ that makes the SRG a powerful alternative to conventional effective interaction methods such as Lee-Suzuki similarity transformations [5].

To date, the SRG applications to nuclear forces have been carried out in free space to construct "soft" nucleon-nucleon (NN) and three-nucleon ($3N$) interactions to be used as input in *ab initio* calculations [5,13]. While the free-space evolution is convenient, as it does not have to be performed for each different nucleus or nuclear matter density, it is necessary to handle $3N$ (and possibly higher-body) interactions to be able to lower the cutoff significantly and maintain approximate cutoff independence of $A \geqslant 3$ observables. The SRG evolution of $3N$ operators represents a significant technical challenge that has only recently been solved in a convenient basis [7].

An interesting alternative is to perform the SRG evolution directly in the A-body system of interest [10–12]. Unlike the free-space evolution, the in-medium SRG (IM-SRG) has the appealing feature that one can

approximately evolve $3, \ldots, A$-body operators using only two-body machinery. The key to this simplification is the use of normal ordering with respect to a finite-density reference state $|\Phi\rangle$. Starting from a general second-quantized Hamiltonian with two- and three-body interactions, all operators can be normal ordered with respect to $|\Phi\rangle$ (e.g., the Hartree-Fock ground state), as opposed to the zero-particle vacuum. Wick's theorem can then be used to exactly write H as

$$H = E_0 + \sum_{ij} f_{ij}\{a_i^\dagger a_j\} + \frac{1}{2!^2}\sum_{ijkl}\Gamma_{ijkl}\{a_i^\dagger a_j^\dagger a_l a_k\} + \frac{1}{3!^2}\sum_{ijklmn} W_{ijklmn}\{a_i^\dagger a_j^\dagger a_k^\dagger a_n a_m a_l\}, \quad (4)$$

where the normal-ordered strings of creation and annihilation operators obey $\langle\Phi|\{a_i^\dagger \cdots a_j\}|\Phi\rangle = 0$, and the normal-ordered 0-, 1-, 2-, and 3-body terms are given by

$$E_0 = \sum_i T_{ii} n_i + \frac{1}{2}\sum_{ij} V^{(2)}_{ijij} n_i n_j + \frac{1}{6}\sum_{ijk} V^{(3)}_{ijkijk} n_i n_j n_k, \quad (5)$$

$$f_{ij} = T_{ij} + \sum_k V^{(2)}_{ikjk} n_k + \frac{1}{2}\sum_{kl} V^{(3)}_{ikljkl} n_k n_l, \quad (6)$$

$$\Gamma_{ijkl} = V^{(2)}_{ijkl} + \frac{1}{4}\sum_m V^{(3)}_{ijmklm} n_m, \quad (7)$$

$$W_{ijklmn} = V^{(3)}_{ijklmn}. \quad (8)$$

Here, the initial n-body interactions are denoted by $V^{(n)}$, and $n_i = \theta(\varepsilon_F - \varepsilon_i)$ are occupation numbers in the reference state $|\Phi\rangle$, with Fermi energy ε_F. It is evident from Eqs. (5)–(7) that the normal-ordered terms, E_0, f, and Γ, include contributions from the three-body interaction $V^{(3)}$ through sums over the occupied single-particle states in the reference state $|\Phi\rangle$. Therefore, truncating the in-medium SRG equations to normal-ordered two-body operators, which we denote by IM-SRG(2), will approximately evolve induced three- and higher-body interactions through the nucleus-dependent 0-, 1-, and 2-body terms. As a preview, we refer to Fig. 1 with the very promising convergence of the ^{4}He ground-state energy, which is comparable to coupled-cluster results.

Using Wick's theorem to evaluate Eq. (2) with $H(s) = E_0(s) + f(s) + \Gamma(s)$ and $\eta = \eta^{(1)} + \eta^{(2)}$ truncated to normal-ordered two-body operators, one obtains the coupled IM-SRG(2) flow equations (with $\bar{n}_i \equiv 1 - n_i$):

$$\frac{dE_0}{ds} = \underline{\sum_{ij}\eta^{(1)}_{ij} f_{ji}(n_i - n_j)} + \frac{1}{2}\sum_{ijkl}\eta^{(2)}_{ijkl}\Gamma_{klij} n_i n_j \bar{n}_k \bar{n}_l, \quad (9)$$

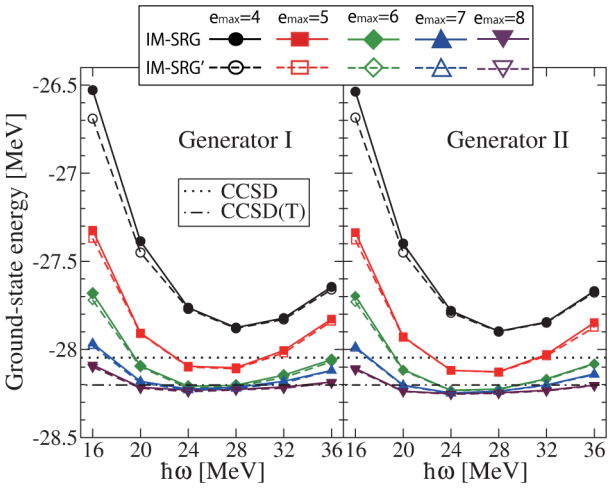

FIG. 1 (color online). Convergence of the in-medium SRG results at the normal-ordered two-body level, IM-SRG(2), for ^{4}He using the generators η^{I} (left) and η^{II} (right panel). The filled (open) symbols correspond to solving Eqs. (9)–(11) with the underlined terms omitted (included). The ground-state energy $E_0(\infty)$ is given as a function of the harmonic oscillator parameter $\hbar\omega$ with increasing single-particle space $e_{\max} \equiv \max(2n + l)$. The initial NN interaction is a free-space SRG-evolved potential with $\lambda = 2.0$ fm^{-1} from the N^{3}LO potential of Ref. [16]. For comparison we show the coupled-cluster CCSD and CCSD(T) energies in the $e_{\max} = 8$ space (calculated at their $\hbar\omega$ minimum).

$$\frac{df_{12}}{ds} = \sum_i[\eta^{(1)}_{1i} f_{i2} + (1 \leftrightarrow 2)] + \underline{\sum_{ij}(n_i - n_j)(\eta^{(1)}_{ij}\Gamma_{j1i2} - f_{ij}\eta^{(2)}_{j1i2})} + \frac{1}{2}\sum_{ijk}[\eta^{(2)}_{k1ij}\Gamma_{ijk2}(n_i n_j \bar{n}_k + \bar{n}_i \bar{n}_j n_k) + (1 \leftrightarrow 2)], \quad (10)$$

$$\frac{d\Gamma_{1234}}{ds} = \sum_i[(\underline{\eta^{(1)}_{1i}\Gamma_{i234}} - f_{1i}\eta^{(2)}_{i234}) - (1 \leftrightarrow 2)] - \sum_i[(\underline{\eta^{(1)}_{i3}\Gamma_{12i4}} - f_{i3}\eta^{(2)}_{12i4}) - (3 \leftrightarrow 4)] + \frac{1}{2}\sum_{ij}[\eta^{(2)}_{12ij}\Gamma_{ij34}(1 - n_i - n_j) + (1,2 \leftrightarrow 3,4)] - \sum_{ij}(n_i - n_j)[(\eta^{(2)}_{j2i4}\Gamma_{i1j3} - \eta^{(2)}_{i1j3}\Gamma_{j2i4}) - (1 \leftrightarrow 2)]. \quad (11)$$

The IM-SRG(2) equations exhibit important similarities to the CCSD approximation of coupled-cluster theory. For instance, the commutator form of the flow equations gives a fully connected structure in which $H(s)$ has at least one contraction with η. Therefore, there are no unlinked diagrams and the flow equations are size extensive. Combined with the $\mathcal{O}(N^6)$ scaling with the number of single-particle orbitals, this makes the method well suited for calculations of medium-mass nuclei. The IM-SRG is intrinsically nonperturbative, where the flow equations,

Eqs. (9)–(11), build up nonperturbative physics via the interference between the particle-particle and the two particle-hole channels for Γ and between the two-particle–one-hole and two-hole–one-particle channels for f. The perturbative analysis reveals that the IM-SRG(2) energy is third-order exact (as is the CCSD approximation) and that f and Γ are second-order exact [14]. It also implies that for calculations with harder interactions, the underlined terms in Eqs. (9)–(11) should be excluded because they produce higher-order contributions (with alternating signs) to E_0 that are also generated by the inclusion of higher-body normal-ordered interactions, $\eta^{(3)}$ and W, corresponding to simultaneous $3p3h$ excitations. Because such triples excitations can be sizable for hard potentials, the underlined terms in Eqs. (9)–(11) should be omitted to better preserve the partial cancellations that would occur against the $[\eta^{(3)}, W]$ contributions. This is consistent with the observation in Fig. 1 that for soft potentials our results are insensitive to the inclusion of these terms. Therefore we define the IM-SRG(2) truncation without these terms.

In this initial study, we restrict our attention to the ground states of doubly magic nuclei and define $H^{od}(s) = f^{\rm od}(s) + \Gamma^{od}(s)$, with

$$f^{od}(s) = \sum_{ph} f_{ph}(s)\{a_p^\dagger a_h\} + \text{H.c.}, \tag{12}$$

$$\Gamma^{od}(s) = \sum_{pp'hh'} \Gamma_{pp'hh'}(s)\{a_p^\dagger a_{p'}^\dagger a_{h'} a_h\} + \text{H.c.}, \tag{13}$$

where p, p' and h, h' denote unoccupied (particle) and occupied (hole) Hartree-Fock orbitals, respectively. We consider two different cases for the generator η. First, we take the Wegner choice $\eta^{\rm I}(s) = [H^d(s), H^{\rm od}(s)]$. Second, we follow White [12] and define

$$\eta^{\rm II} = \sum_{ph} \frac{f_{ph}\{a_p^\dagger a_h\}}{f_p - f_h - \Gamma_{phph}} - \text{H.c.} + \sum_{pp'hh'} \frac{\Gamma_{pp'hh'}\{a_p^\dagger a_{p'}^\dagger a_{h'} a_h\}}{f_p + f_{p'} - f_h - f_{h'} + A_{pp'hh'}} - \text{H.c.}, \tag{14}$$

where $A_{pp'hh'} = \Gamma_{pp'pp'} + \Gamma_{hh'hh'} - \Gamma_{phph} - \Gamma_{p'h'p'h'} - \Gamma_{ph'ph'} - \Gamma_{p'hp'h}$ and $f_p \equiv f_{pp}$ (the s dependence is suppressed for simplicity). Both generators suppress off-diagonal ($1p1h$ and $2p2h$) couplings and drive the Hamiltonian towards diagonal form,

$$H(\infty) = E_0(\infty) + f^d(\infty) + \Gamma^d(\infty), \tag{15}$$

but White's generator ($\eta^{\rm II}$) is significantly more efficient, because the flow equations are less stiff in this case and the evaluation of η at each step is significantly faster. The evolved Hamiltonians using $\eta^{\rm I}$ and $\eta^{\rm II}$ are unitarily equivalent if no truncations are made. Any differences in energy eigenvalues therefore provide a measure of the truncation error resulting from neglected three- and higher-body normal-ordered terms in our calculations.

At the end of the flow, the reference state becomes the ground state of $H(\infty)$, with fully interacting ground-state energy $E_0(\infty)$, and $|\Phi\rangle$ decouples from the rest of the Hilbert space ($1p1h, 2p2h, \ldots, ApAh$ sectors),

$$QH(\infty)P = 0 \quad \text{and} \quad PH(\infty)Q = 0, \tag{16}$$

where $P = |\Phi\rangle\langle\Phi|$ and $Q = 1 - P$. This decoupling follows from the observation that all other normal-ordered couplings annihilate the reference state, $[f^d(s) + \Gamma^d(s)]|\Phi\rangle = 0$. Combined with $f^{od}(\infty)$ and $\Gamma^{od}(\infty)$ being driven to zero, this implies the block-diagonal structure of Eq. (16). The IM-SRG is very flexible and alternative choices of H^{od} (and η) can be used to target excited states, single-particle properties, and to construct effective interactions and operators for open-shell systems [11,12].

Figure 1 shows the IM-SRG(2) ground-state energy $E_0(\infty)$ for ^{4}He calculated in increasing spaces defined by the single-particle $e_{\rm max} \equiv \max(2n + l)$. For all cases the flow equations, Eqs. (9)–(11), were solved in a jj-coupled basis. The $\eta^{\rm I}$ and $\eta^{\rm II}$ results agree within 20 keV, which suggests the truncation to normal-ordered two-body interactions is a controlled approximation. This is consistent with Fermi system arguments for interparticle interactions where a finite-density reference state is close to the interacting ground state [15]. In addition, the IM-SRG(2) $e_{\rm max} = 8$ energy is essentially converged and within 20 keV of the exact NCSM diagonalization [7], and in good agreement with the coupled-cluster CCSD(T) energies (based on the code of Ref. [3]). We stress that the agreement is obtained at the normal-ordered two-body level without including residual three-body interactions.

The suppression of $H^{od}(s)$ is illustrated in Fig. 2, which shows the $\eta^{\rm I}$ evolution of normal-ordered two-body matrix elements Γ_{ijkl}. As expected, the off-diagonal couplings ($ijkl = pphh$ or $hhpp$) are rapidly driven to zero. An important practical consequence is that many-body approximations become more effective under the SRG evolution before complete decoupling has been reached.

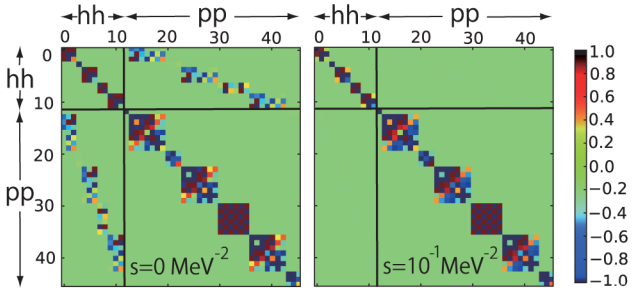

FIG. 2 (color online). In-medium SRG evolution of normal-ordered two-body matrix elements Γ_{ijkl} connecting hole-hole (hh) and particle-particle (pp) states for ^{16}O starting from a smooth-cutoff $V_{\rm low}k$ with $\Lambda = 1.8$ fm^{-1}. The color scale is in MeV, and initial and s-evolved results are shown. The axes label two-body jj-coupled states $|(n_a, l_a, j_a, t_{z_a}), (n_b, l_b, j_b, t_{z_b}); J = 0\rangle$. The Γ_{ijkl} where $ijkl = ppph$ or $hhhp$, which are not driven to zero with the current generator, are not shown.

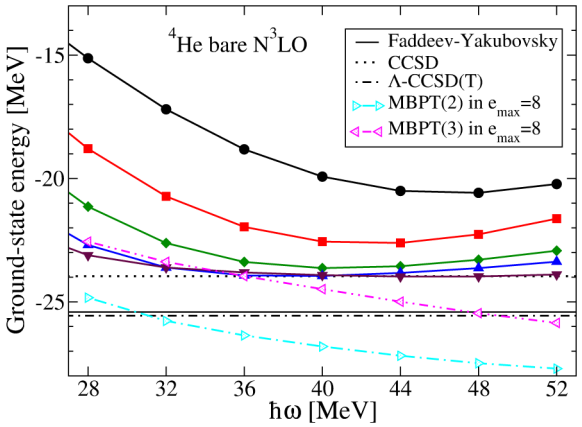

FIG. 3 (color online). Convergence of the IM-SRG(2) energy $E_0(\infty)$ for ^{4}He using the generator η^{II} and starting from the "bare" N^{3}LO potential of Ref. [16]. The notation is the same as in Fig. 1. The converged IM-SRG(2) energy agrees well with the CCSD result (the coupled-cluster energies are taken from Ref. [3]), while second- and third-order many-body perturbation theory, MBPT(2) and MBPT(3), clearly break down.

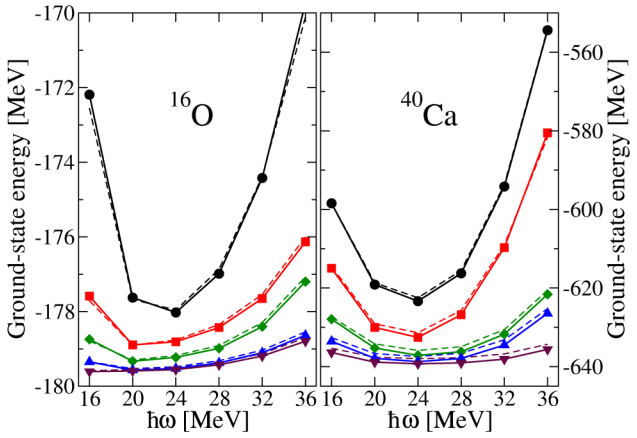

FIG. 4 (color online). Convergence of the IM-SRG(2) energy $E_0(\infty)$ for ^{16}O (left) and ^{40}Ca (right panel) using the generator η^{II} (solid symbols) and in comparison to CCSD results (dashed lines). The notation is the same as in Fig. 1. The initial V_{NN} is a smooth-cutoff $V_{\mathrm{low}\,k}$ with $\Lambda = 1.8$ fm^{-1} for ^{16}O and a free-space SRG potential with $\lambda = 1.8$ fm^{-1} for ^{40}Ca, both evolved from the N^{3}LO potential of Ref. [16].

Figure 3 shows the IM-SRG(2) results for ^{4}He starting from a "bare" N^{3}LO potential, which is a harder initial interaction. The ground-state energy clearly converges to a value close to the CCSD result. The failure of many-body perturbation theory in this case verifies that the IM-SRG is an intrinsically nonperturbative method.

Finally, we apply the IM-SRG to calculate the ground-state energies of ^{16}O and ^{40}Ca in Fig. 4 starting from low-momentum interactions. As for the ^{4}He results of Fig. 3, the calculations are well converged and have accuracies that closely track the CCSD energies. As discussed above, the IM-SRG(2) includes some simultaneous $3p3h$ excitations for $E_0(s)$ that partially cancel against contributions that would arise if normal-ordered three-body operators were kept in the flow equations. This motivated excluding the underlined terms in Eqs. (9)–(11). The omitted terms are negligible for soft interactions, as shown in Fig. 1, but they become larger for hard interactions such as the "bare" N^{3}LO potential used here, and thus require a consistent treatment either by omitting them in the IM-SRG(2) equations, or by including normal-ordered three-body operators in the flow equations. In the former case, we find here an accuracy that is comparable to CCSD calculations.

In summary, we have shown that the in-medium SRG is a promising method for *ab initio* calculations of light and medium-mass nuclei. The use of normal ordering allowed us to evolve the dominant induced $3, \ldots, A$-body interactions using only two-body machinery. We have presented first IM-SRG(2) results for the ground-state energies of closed-shell nuclei, which were in very good agreement with CC calculations. Work is in progress to include $3N$ forces and to study effective valence shell-model Hamiltonians for open-shell systems. The same IM-SRG flow equations apply to the normal-ordered 0-, 1-, and 2-body parts of operators.

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