Similarity renormalization group and many-body effects in multiparticle systems

Kristina D. Launey, Tomáš Dytrych, and Jerry P. Draayer

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Similarity Renormalization Group and Many-body Effects in Multi-particle Systems

Kristina D. Launey, Tomáš Dytrych, and Jerry P. Draayer
Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

The similarity renormalization group (SRG), based on the simple one-body free harmonic oscillator Hamiltonian, is applied to various nucleon-nucleon realistic interactions to investigate the unitarity of the SRG transformations. Two-body and three-body contributions to the SRG-evolved Hamiltonian are studied in the framework of spectral distribution theory for reasonable SRG cutoffs and in multi-particle systems, with up through 28 particles considered. The outcome points to the first evidence for the overall importance of 3-body SRG-induced interactions and especially, of its 2-body effective content in multi-nucleon systems, without the need for large-scale shell model calculations for many light to heavier nuclei.

I. INTRODUCTION

The similarity renormalization group (SRG) approach [1, 2] to internucleon interactions aims to achieve a softer (renormalized) interaction [3, 4] that enables the use of manageable model spaces within the framework of modern *ab initio* shell model studies (e.g., [5–8]). These models, in turn, can be invoked to provide accurate descriptions of light, and ultimately even heavier nuclei. The $H_{\rm eff}$ renormalized interaction is obtained via continuous unitary transformations of the original realistic Hamiltonian and is thus equivalent to the original one, provided that the $H_{\rm eff}$ includes all the nonnegligible many-body SRG-generated terms. Clearly, if the latter are only of low particle rank, say up to three-body, then a three-particle ($a = 3$) model space can be employed for the SRG evolution (SRG^a), and model-independent unitarity of the result is assured. Furthermore, such an SRG^a-evolved interaction can be used for *ab initio* descriptions for nuclei of mass numbers $A \geq a$. This places a premium on the study of and estimates for the significance of many-body terms generated throughout an SRG evolution, both in few-body systems ($a \lesssim 3$) as well as in many-nucleon systems, such as $a \sim 12 - 16$ that are of interest to current *ab initio* shell model studies.

In this paper, we present results for SRG evolutions in multi-particle systems, $2 \leq a \leq 28$. We focus on the most dominant SRG-induced many-body contribution. We have shown [9] that it is generated at the very beginning of the SRG flow, namely, by the double commutator $H_0' = [[C, H_0], H_0]$. For a 1-body SRG operator C and a 2-body initial Hamiltonian $H_0 = H_{NN}$, H_0' includes up to 3-body terms. We have also shown in [9] that for flows not infinitely evolved (as for decoupling parameters λ_d used in practical applications), the overall contribution of other SRG-induced terms practically results in only varying the strength of H_0'. This could be also understood by the fact that SRG-induced terms, which rapidly decrease in strength with the flow, project almost entirely onto H_0' during the initial stage of the flow when the low-lying eigenvalues of H_0 are affected most. Therefore, by studying the many-body content of the first SRG-induced term in an a-particle system, we examine the nonnegligible many-body induced contributions to the SRG^a-evolved Hamiltonian. In this analysis we take a from 2 up to 28 particles, which is more than sufficient to demonstrate the effect of the evolution with increasing number of particles.

The present analysis are carried forward within the framework of spectral distribution theory (SDT) [10–12] (see [13], for a review on SDT), where, e.g., a three-body interaction can be straightforwardly cast into a sum of 'density-dependent' monopole (centroid), one-body (induced single-particle energies), and two-body parts together with its residual, irreducible three-body part. It is interesting to note that SDT provides an easy-to-follow prescription – readily extensible to 4-body interactions and beyond – on how to extract these parts and furthermore, on how they propagate with the number of nucleons (as shown in Appendix A). This information is of special interest when three-body (or higher rank) interactions are invoked (e.g., [14–16]).

The outcome of the present study offers the first evidence for the overall importance of 3-body SRG-induced interactions (when a 1-body C is employed) for a range of nuclei that reaches beyond the lightest few-nucleon systems. The effect of neglecting these interactions is also studied. This is achieved without the need for carrying out large-scale shell model calculations for many light to heavier nuclei. It also goes beyond the information a few low-lying energy states could provide by treating the full Hamiltonian and its many-body terms in their entirety at an operator level. This ensures the extensibility of the results as it relates to the influence of the induced many-body interaction on a broad variety of spectral observables, as well as on Hamiltonian eigenstates, and points toward a means for studying the effect of the renormalization on related observables (e.g., transition rates). We note that for the purpose of this study, namely to explore the overall significance of the many-body contributions to the SRG-induced interactions, only low-order energy moments are sufficient (e.g., the second-order moment of an interaction that yields its strength). Nonetheless, if one were to include higher-order energy moments that are typically much less important to the low-energy nuclear dynamics, one would obtain more detailed results that, in principle, should enable a reproduction of all observables associated with conventional microscopic analyses.

II. SRG-INDUCED MANY-BODY INTERACTIONS

The SRG has been designed as a nonperturbative method that performs a continuous sequence of unitary transformations of a H Hamiltonian, $H_s = U(s) H U^\dagger(s)$, yielding the following class of equations [1, 2],

$$\frac{d}{ds} H_s = [\eta_s, H_s] = [[C, H_s], H_s], \tag{1}$$

where C can be any hermitian operator, which in turn defines the antihermitian $\eta_s = [C, H_s]$ generator and the $U(s)$ transformation ($\eta_s = \frac{dU(s)}{ds} U(s)^\dagger$). If C is chosen to be diagonal in the representation of the initial H, H_s is driven toward a (block-)diagonal form in this representation with decreasing "decoupling" energy parameter $\lambda_d = 1/\sqrt{s}$.

The present study and the analysis of its outcome refer to a one-body C and a two-body H_0 initial Hamiltonian. Let $a_i^{(\dagger)}$ denote the fermion annihilation (creation) operator, which destroys (creates) a fermion in a state labeled by a set of quantum numbers i. Then, for a diagonal 1-body C, $C = \sum_i C_i a_i^\dagger a_i$, and a 2-body $H_0 = \frac{1}{(2!)^2} \sum_{ijkl} V_{ijkl} a_i^\dagger a_j^\dagger a_l a_k$, the initial transformation yields a change in H_0 given by Eq. (1),

$$\begin{aligned}
\left.\frac{d}{ds} H_s\right|_{s=0} &= [\eta_0, H_0] = [[C, H_0], H_0] = \frac{1}{16} \sum_{ijrs} a_i^\dagger a_j^\dagger \\
&\times \left(2 \sum_{kl} (C_i + C_j + C_r + C_s - 2C_k - 2C_l) V_{ijkl} V_{klrs} \right. \\
&+ \left. 4 \sum_{lkq} (C_i + C_j + C_r + C_s - C_k - C_q - 2C_l) V_{ijkl} V_{lqrs} a_q^\dagger a_k \right) a_s a_r \\
&= \frac{1}{4} \sum_{ijrs} W_{ijrs} a_i^\dagger a_j^\dagger a_s a_r + \frac{1}{4} \sum_{ijkrsq} W^{NA}_{ijqrsk} a_i^\dagger a_j^\dagger a_q^\dagger a_k a_s a_r \\
&= H_I^{\rm 2b} + H_I^{\rm 3b}.
\end{aligned} \tag{2}$$

The first term, $H_I^{\rm 2b}$, realizes the two-body contribution to the SRG-induced interaction with matrix elements,

$$W_{ijrs} = \tfrac{1}{2} \textstyle\sum_{kl} (C_i + C_j + C_r + C_s - 2C_k - 2C_l) V_{ijkl} V_{klrs}, \tag{3}$$

while the second term, $H_I^{\rm 3b}$, introduces a three-body interaction given by non-antisymmetrized matrix elements,

$$W^{NA}_{ijqrsk} = -\sum_l (C_i + C_j + C_r + C_s - C_k - C_q - 2C_l) V_{ijkl} V_{qlrs}, \tag{4}$$

with the corresponding antisymmetrized ones written as,

$$\begin{aligned}
W_{ijqrsk} &= W^{NA}_{ijqrsk} - W^{NA}_{ijqrks} - W^{NA}_{ijqksr} \\
&- W^{NA}_{iqjrsk} + W^{NA}_{iqjrks} + W^{NA}_{iqjksr} \\
&- W^{NA}_{qjirsk} + W^{NA}_{qjirks} + W^{NA}_{qjiksr}.
\end{aligned} \tag{5}$$

For finite flows evolved to reasonable λ_d, the $[\eta_0, H_0]$ initial SRG-induced interaction of Eq. (2) constitutes the predominant contribution to the total SRG-induced interaction [9]. Indeed, while higher-order SRG-induced terms may be important, each of these terms can be expressed as a sum of an interaction of the $[\eta_0, H_0]$ kind and higher-particle rank interactions. The latter can be controlled to be negligible [9]. It is thus clear that the higher-order SRG-induced terms, if found significant, can only affect the overall $[\eta_0, H_0]$ strength, that is, the magnitude of the total induced interaction, without introducing appreciable mixing of interactions of other kinds or of higher particle ranks. Therefore, for a 1-body C and a 2-body H_0, it is sufficient to study the 2-body ($H_I^{(2b)}$) and 3-body ($H_I^{(3b)}$) content of the $[\eta_0, H_0]$ SRG-induced term (2), as well as its role in many-particle systems. This, in turn, provides information about the dominant many-body contributions within a many-body SRG-evolved Hamiltonian.

If Eq. (1) is applied to operators in a matrix representation associated with the many-body basis space of a particles (SRG^a), then for $a = 2$, the $H_I^{\rm 2b}$ interaction is the only term that contributes to the total SRG-induced interaction. However, when the SRG evolution is performed within a general a-particle basis ($a \geq 3$), the $H_I^{\rm 3b}$ interaction is needed and together with $H_I^{\rm 2b}$ (and negligible SRG-induced interactions of a higher particle rank) assures the unitarity of the SRG transformations. The contribution of the $H_I^{\rm 3b}$ to the total SRG^a-induced interaction can be evaluated based on the $H_I^{\rm 3b}$ properties between all possible triples formed by the a particles. Such a study, which encompasses SRG evolutions for systems with a large number of particles – in the case of this paper, up through $a = 28$, is made possible in the framework of spectral distribution theory.

III. SPECTRAL DISTRIBUTION THEORY AND DERIVATION OF 'DENSITY-DEPENDENT' TERMS

Spectral distribution theory (SDT) [10–12, 17] originated as an alternative microscopic approach to the conventional shell model technique. The efficacy of the theory stems from the fact that typically low-order energy moments dominate the many-particle spectroscopy as a result of leading surviving features of the underlying microscopic interaction. Convergence to the shell-model results improves as higher-order energy moments are taken into account or toward the limit of many particles occupying a much larger available single-particle space. The theory also provides the means to calculate important average contributions, nuclear level densities, degree of symmetry violation, as well as various measures. The SDT approach has been successfully applied to studies of energy spectra and reactions for p-, sd, and fp-shell nuclei [18–23], as well as for understanding dominant features and differences among sd-shell realistic effective interactions [24, 25]. Recent applications include explorations on quantum chaos, nuclear structure, and parity/time-reversal violation (for example, see [13, 26–30]). In the present study, we do not utilize the SDT microscopic approach but rather make use of tools developed in SDT. Specifically, we employ second-order energy moments widely used as measures of the overall strength of an interaction and its similarity to other interactions.

In SDT, for an arbitrary basis of dimension N_d the traceless (many-body) Hamiltonian matrix representation can be mapped onto a vector in a multi-dimensional linear vector space. The σ_H vector "length" (specifying the interaction "strength") is related to the Hilbert-Schmidt norm,

$$\sigma_H^2 = \langle (H - \langle H \rangle)^\dagger (H - \langle H \rangle) \rangle \tag{6}$$

with $\langle \ldots \rangle \equiv \frac{1}{N_d}\mathrm{Tr}(\ldots)$, while the spatial orientation of two operators, H and H', is given by their correlation coefficient (specifying the similarity between the two interactions),

$$\zeta_{H,H'} = \frac{\langle (H - \langle H \rangle)^\dagger (H' - \langle H' \rangle) \rangle}{\sigma_H \sigma'_H} = \cos\theta \tag{7}$$

with θ being the angle between H and H'. Hence, σ_H is a natural measure of the H operator size and realizes the spread of the H eigenvalue distribution. As is well-known, the smaller the σ_H (the weaker the interaction), the more compressed the energy spectrum of H and the smaller its effect on the $(H + H')$ spectrum for a much stronger H' [11].

Furthermore, SDT provides a tool to express an interaction of a particle rank k – e.g., $k = 3$ for the $H_I^{3\mathrm{b}}$ in Eq. (2) – in terms of $\mathcal{H}^{(k)}(\nu)$ interactions of a definite particle rank ν for an A-particle system,

$$H(k) = \sum_{\nu=0}^{k} \binom{A-\nu}{k-\nu} \mathcal{H}^{(k)}(\nu). \tag{8}$$

The $\mathcal{H}^{(k)}(\nu)$ are also called "pure" ν-body interactions. For example, for a scalar distribution over a single-particle basis space of dimension $\mathcal{N}$, the $\mathcal{H}^{(k)}(\nu)$ is an U($\mathcal{N}$) irreducible tensor of rank $\nu = 0, 1, \ldots, k$, for a k-body interaction. From a physical point of view, this expansion realizes contributions to the $H(k)$ interaction from 'density-dependent' ν-body terms with, e.g., $\nu = 0$ and $\nu = 1$ giving the vacuum expectation value and the 'density-dependent' mean field, respectively.

In what follows, we will use a scalar distribution, which invokes averages over all single-particle basis states.

A. Two-body interactions

For a two-body interaction as given in [12], the monopole moment (centroid), which is the average expectation value, is defined in the scalar case as,

$$W_c^{(2)} = \frac{1}{\binom{\mathcal{N}}{2}} \sum_{r<s} W_{rsrs} = \frac{\sum_{rs} W_{rsrs}}{\mathcal{N}(\mathcal{N}-1)}, \tag{9}$$

where $\mathcal{N}$ is the dimensionality of the single-particle model space and $\binom{\mathcal{N}}{2} = \sum_{r<s} 1$. For a spherical harmonic oscillator (HO) basis (m-scheme) of like particles, $\mathcal{N} = \sum_\eta (\eta+1)(\eta+2)$, where η is the oscillator shell quantum number.

Contraction of the two-body interaction into an effective one-body operator under the particular group structure yields the effective mean field contribution, sometimes referred as induced single-particle energies,

$$\lambda_{rt}^{(2)} = \frac{1}{\mathcal{N}-2} \sum_s W_{rsts} \tag{10}$$

with their traceless counterparts given as,

$$\tilde{\lambda}_{rt}^{(2)} = \lambda_{rt}^{(2)} - \delta_{rt} \frac{1}{\mathcal{N}} \sum_s \lambda_{ss}^{(2)} = \lambda_{rt}^{(2)} - \delta_{rt} \frac{\mathcal{N}-1}{\mathcal{N}-2} W_c^{(2)}. \tag{11}$$

Hence, the traceless pure two-body matrix elements are defined as,

$$\begin{aligned} \tilde{v}_{rstu}^{(2)} = W_{rstu} &- (\tilde{\lambda}_{rt}^{(2)} \delta_{su} + \tilde{\lambda}_{su}^{(2)} \delta_{rt} - \tilde{\lambda}_{ru}^{(2)} \delta_{st} - \tilde{\lambda}_{st}^{(2)} \delta_{ru}) \\ &- W_c^{(2)} (\delta_{rt}\delta_{su} - \delta_{ru}\delta_{st}). \end{aligned} \tag{12}$$

For A particles, which interact through a two-body interaction $H(2)$, the strength of the interaction reflects its propagation in the many-particle systems and is given as,

$$\sigma^2_{H(2)}(A) = \mathcal{P}(1,A)\sum_{ir}(A-1)^2\tilde{\lambda}^{(2)}_{ir}\tilde{\lambda}^{(2)}_{ir} + \mathcal{P}(2,A)\sum_{i<j,k<l}\tilde{v}^{(2)}_{ijkl}\tilde{v}^{(2)}_{ijkl} \tag{13}$$

with $\mathcal{N}$-dependent propagation functions,

$$\mathcal{P}(\nu,A) = \frac{\binom{A}{\nu}}{\binom{\mathcal{N}}{\nu}}\frac{\binom{\mathcal{N}-A}{\nu}}{\binom{\mathcal{N}-\nu}{\nu}}. \tag{14}$$

Note that $\sigma_{H(2)}(A)$ (13) depends only on sums calculated for the two-body system and is exactly equal to $\sigma_{H(A)}$ that can be calculated by constructing the corresponding many-body $H(A)$ Hamiltonian and using Eq. (6) with $H(A)$.

B. Three-body interactions

We use the SDT method outlined in [12] and apply it to a 3-body interaction to derive its pure interactions of a particle rank 1, 2, and 3 under the space partitioning in consideration, namely, the scalar distribution (Appendix A). The monopole moment (centroid) is thus defined as,

$$W^{(3)}_c = \frac{1}{\binom{\mathcal{N}}{3}}\sum_{i<j<q}W_{ijqijq} = \frac{\sum_{ijq}W_{ijqijq}}{\mathcal{N}(\mathcal{N}-1)(\mathcal{N}-2)}, \tag{15}$$

where $\binom{\mathcal{N}}{3} = \sum_{i<j<q}1$. The effective one-body interaction is given in terms of,

$$\lambda^{(3)}_{ir} = \frac{1}{\binom{\mathcal{N}-2}{2}}\sum_{j<q}W_{ijqrjq} = \frac{1}{(\mathcal{N}-2)(\mathcal{N}-3)}\sum_{jq}W_{ijqrjq} \tag{16}$$

with the corresponding interaction of a particle rank one (traceless mean-field contribution) defined by means of,

$$\tilde{\lambda}^{(3)}_{rt} = \lambda^{(3)}_{rt} - \delta_{rt}\frac{1}{\mathcal{N}}\sum_s\lambda^{(3)}_{ss} = \lambda^{(3)}_{rt} - \delta_{rt}\frac{\mathcal{N}-1}{\mathcal{N}-3}W^{(3)}_c. \tag{17}$$

The two-body matrix elements, constructed by contraction of the 3-body interaction,

$$v^{(3)}_{ijrs} = \frac{1}{\mathcal{N}-4}\sum_q W_{ijqrsq} \tag{18}$$

yield, in turn, the matrix elements of the pure 2-body $\mathcal{H}^{(3)}(2)$,

$$\tilde{v}^{(3)}_{rstu} = v^{(3)}_{rstu} - \frac{\mathcal{N}-3}{\mathcal{N}-4}(\tilde{\lambda}^{(3)}_{rt}\delta_{su} + \tilde{\lambda}^{(3)}_{su}\delta_{rt} - \tilde{\lambda}^{(3)}_{ru}\delta_{st} - \tilde{\lambda}^{(3)}_{st}\delta_{ru}) - \frac{\mathcal{N}-2}{\mathcal{N}-4}W^{(3)}_c(\delta_{rt}\delta_{su} - \delta_{ru}\delta_{st}). \tag{19}$$

For A particles, the strength of an interaction that is up to three-body is given as,

$$\sigma^2_{H(1+2+3)}(A) = \mathcal{P}(1,A)\sum_{ir}\left(\tilde{\lambda}^{(1)}_{ir} + (A-1)\tilde{\lambda}^{(2)}_{ir} + \binom{A-1}{2}\tilde{\lambda}^{(3)}_{ir}\right)^2 + \mathcal{P}(2,A)\sum_{i<j,k<l}\left(\tilde{v}^{(2)}_{ijkl} + (A-2)\tilde{v}^{(3)}_{ijkl}\right)^2 + \mathcal{P}(3,A)\sum_{i<j<q,r<s<k}\tilde{w}^{(3)}_{ijqrsk}\tilde{w}^{(3)}_{ijqrsk}, \tag{20}$$

where the $\mathcal{N}$-dependent $\mathcal{P}$ propagation functions are given in Eq. (14), as well as $\tilde{\lambda}^{(1)}_{ii} = \lambda^{(1)}_{ii} - \frac{1}{\mathcal{N}}\sum_s\lambda^{(1)}_{ss}$ are related to $\lambda^{(1)}_{ii}$ single-particle energies (if used in the model at hand). The explicit construction of the pure three-body matrix elements $w^{(3)}_{ijqrsk}$ is not required to evaluate the $w^{(3)}_{ijqrsk}$-dependent sum in the last term of Eq. (20). This sum can be calculated using Eq. (20) for $A = 3$ and that $\sigma^2_{H(3)}(3) = \binom{\mathcal{N}}{3}^{-1}\sum_{i<j<q,r<s<k}W_{ijqrsk}W_{ijqrsk}$ is known. Clearly, $\sigma^2_{H(3)}(A)$ follows from Eq. (20) with $\tilde{\lambda}^{(1)}_{ir}$, $\tilde{\lambda}^{(2)}_{ir}$, and $\tilde{v}^{(2)}_{ijkl}$ set to zero.

In the present study, the 'density-dependent' one-body and two-body parts of the $H^{(3b)}_{\rm I}$ 3-body interaction are calculated using Eq. (17) and Eq. (19), respectively. If the pure 3-body contribution to the $H^{(3b)}_{\rm I}$ is found to be insignificant for the description of certain spectral features, these equations offer a straightforward approach to extract from the $H^{(3b)}_{\rm I}$ its one- and two-body parts and thus, simplifying the problem to one utilizing a 2-body

TABLE I: SRG-induced interactions and the corresponding notations used in the paper. The interactions $H_{\rm I}^{(2b)}$ and $H_{\rm I}^{(3b)}$ are derived using Eqs. (3-5). The $H_{\rm I,2b}^{(3b)}$ includes pure one- and two-body interactions with matrix elements calculated using Eq. (17) and Eq. (19), respectively, for the 3-body $H_{\rm I}^{(3b)}$.

2-body induced, $H_{\rm I}^{(2b)}$		total 2-body induced, $H_{\rm I,2b}^{\rm tot}$	total induced, $H_{\rm I}^{\rm tot}$
3-body induced, $H_{\rm I}^{(3b)}$	2-body of 3-body induced, $H_{\rm I,2b}^{(3b)}$		
	pure 3-body of 3-body induced, $H_{\rm I,3b}^{(3b)}$		

SRG-evolved interaction. The various SRG-induced interactions and their notations used throughout the paper are given in Table I.

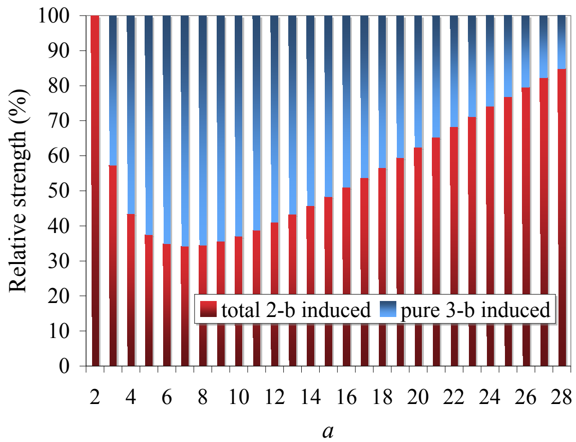

FIG. 1: (Color online) Contributions of the $H_{I,2b}^{tot}$ total 2-body SRG-induced interaction (red lower bars) and of the $H_{I,3b}^{(3b)}$ pure 3-body SRG-induced interaction (blue upper bars) to the total SRG-induced interaction as a function of the a number of particles in the many-body basis space for $\rm N^3LO$ interaction and 10 j-levels. Similar results are obtained for JISP16.

parameter $\hbar\omega = 11$ MeV) [33] and JISP16 (15 MeV) [34], as well as, for illustration, CD-Bonn (15 MeV) [35] and AV18 (18 MeV) [36], in an m-scheme basis for six to ten j-levels ($0s_{1/2}$, $0p_{1/2}$, $0p_{3/2}$, $1s_{1/2}$, $0d_{3/2}$, $0d_{5/2}$, $1p_{1/2}$, $1p_{3/2}$, $0f_{5/2}$, and $0f_{7/2}$) and for like particles. As shown below, these model spaces already reveal a convergence trend for the quantities studied here. This, together with the similar patterns observed when random interactions are employed, brings forward results that are not significantly restricted by the choice of interactions or model spaces. In addition, while studies of the important $T = 0$ part of the interactions are needed and underway, the present investigation focuses on the $T = 1$ part, which yields three-body interactions that are comparatively simpler to handle. Such a restriction is expected not to alter the present conclusions, because − even though there are strong detailed differences − the overall features relevant to this study for both $T = 0$ and $T = 1$ parts are very similar. For example, for ten j-levels up through the pf shell, the strength of the $T = 0$ ($T = 1$) $\rm N^3LO$ NN interaction is 2.84 MeV (1.65 MeV) with a strength of its pure one-body part being 0.33 MeV (0.19 MeV) and of its monopole part being −0.82 MeV (−0.44 MeV). This together with a correlation of the interaction to the $C = H_{\rm HO}$ SRG operator of 0.103 for $T = 0$ and 0.093 for $T = 1$ shows that no large discrepancies are expected for the $T = 0$ and $T = 1$ results.

IV. APPLICATION OF SRG RENORMALIZED INTERACTIONS TO HEAVIER NUCLEI

A. Model description

While the SRG renormalization of NN or NNN interactions is typically restricted to a 2- or 3-particle model space [31, 32] and furthermore, most many-body SRG-induced interactions are impossible to handle, the SDT framework presented above provides a straightforward approach to investigate the overall role of the SRG-generated interactions for evolutions in model spaces of larger particle numbers, e.g., out to $a = 28$ in the current study. We apply the SRG procedure (Eq. 1) using the free HO Hamiltonian $C = H_{\rm HO}$ (one-body) to various realistic NN interactions H_0, namely, $\rm N^3LO$ (HO

As previously mentioned, it is sufficient, without neglecting any significant SRG-induced terms, to study the 2-body ($H_I^{(2b)}$) and 3-body ($H_I^{(3b)}$) SRG-induced terms defined in (2). The effect these interactions have for SRG evolutions performed for $a \geq 3$, is calculated using Eqs. (13) and (20), which reflect the overall properties of the many-body Hamiltonian for a particles that interact through 2-body and 3-body interactions. In particular, first, we show the role of the pure 3-body interactions ($H_{I,3b}^{(3b)}$) for SRG evolutions in a model space of $3 \leq a \leq 28$ particles. We also study the 2-body part $H_{I,2b}^{(3b)}$ that emerges from the $H_I^{(3b)}$ term. Finally, we compare full $\rm SRG^a$ calculations (excluding negligible higher-order SRG-induced terms) to the case of omitting the $H_I^{(3b)}$ term (equally, employing an $\rm SRG^{a=2}$ flow) and show the effect it has on the SRG-evolved interaction.

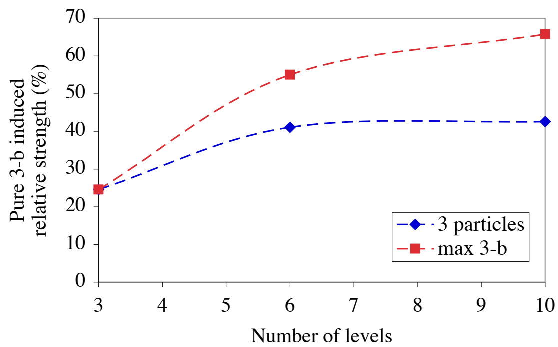

FIG. 2: (Color online) Contribution of the $H_{I,3b}^{(3b)}$ pure 3-b SRG-induced interaction to the total SRG-induced interaction for N^{3}LO as a function of the number of j-levels considered. The maximum contribution among systems of $3 \leq a \leq 38$ particles is shown (red squares) together with the contribution within a 3-particle system (blue diamonds).

B. Results and discussions

The analysis of the results reveals that for an SRG evolution performed in a three-particle ($a = 3$) system, 2-body interactions ($H_{I,2b}^{tot}$) – those that realize the combined contribution of the 2-body induced $H_I^{(2b)}$ and the $H_{I,2b}^{(3b)}$ 2-b part of the 3-b induced term – account for $\sim 60\%$ of the total SRG-induced interaction (Fig. 1, red lower bars, $a = 3$). For example, for N^{3}LO, this portion is 57.4% for four HO shells (10 j-levels) and 58.9% for three HO shells (similarly, 55.9% for JISP16). Equally, only $\sim 40\%$ is realized by the pure 3-b interactions, $H_{I,3b}^{(3b)}$ (Fig. 1, blue upper bars, $a = 3$). As shown in Fig. 1, this 3-body contribution first increases with increasing number of particles to $\sim 2/3$ of the total induced interaction, and beyond this, steadily decreases as more particles fill up the model space. These features, we find, have already exhibited a tendency toward convergence for the 10-level model space considered (Fig. 2). The induced $H_{I,2b}^{tot}$ and the initial H_{NN} 2-body interactions thus comprise the dominant contribution to the SRG-evolved Hamiltonian. This remarkable result points to the fact that the renormalized interaction is essentially two-body driven for any a-particle system.

Note that the dominating 2-body portion shown in Fig. 1 includes a 2-body contribution, $H_{I,2b}^{(3b)}$, from the 3-b SRG-induced term of Eq. (2), which is not accounted for in an SRG$^{a=2}$ flow. However, our findings reveal that the role this contribution plays in an SRG-evolved interaction is considerable and even dominant for heavier systems (Fig. 3, magenta dotted vectors). This is in agreement with additional evidence for the need of an SRG$^{a=3}$ flow based on observations of low-lying state energies in a few light nuclei [16, 31, 32], but the systematic importance of the 2-body content of the 3-body induced terms has not been detected heretofore. Fig. 3 displays a vector representation of the SRG-induced interactions under consideration (Table I) for an SRG evolution performed for representative model spaces. Namely, we show model spaces of $a = 3$, $a = 6$ (around the maximum contribution of the pure 3-body interaction to the total induced one) and $a = 12$ particles. The total 2-body SRG-induced interaction, which is shown in Fig. 1 as red (lower) bars, is represented in Fig. 3 by a red (dashed) vector, which is made up of the 2-body induced $H_I^{(2b)}$ (a purple vector in the horizontal plane) and the $H_{I,2b}^{(3b)}$. The latter together with the pure 3-body interaction (blue vector along the vertical axis) make up the $H_I^{(3b)}$ 3-b SRG-induced term, which, in turn, adds up to $H_I^{(2b)}$ to yield – according to Eq. (2) – the total SRG-induced interaction (black vector in Fig. 3). Higher-order SRG-induced terms, if found nonnegligible, have an overall significant effect only on the axis scale (different vector lengths). As manifested in Fig. 3, while $H_{I,2b}^{(3b)}$ plays a negligible role for $a = 3$ particles, its contribution is essential and, for larger a, is comparable to or even larger than the $H_I^{(2b)}$. This points to the fact that the three-body induced interactions, and especially their 'density-dependent' 2-body content, that are not accounted for in an $a = 2$ SRG evolution of a H_{NN} play an essential role in describing heavier systems using such SRG-renormalized interactions.

It is important to further explore $H_I^{(2b)}$ and H_I^{tot}. $H_I^{(2b)}$ is the total SRG$^{a=2}$-induced interaction that yields an SRG-renormalized interaction no longer unitarily equivalent to the original one for $A > 3$ nuclei. H_I^{tot} is the total induced interaction, which retains the unitarity. As shown in Figure 3, even though both interactions typically have a comparable strength, they are actually expected to render quite different spectral features. This is manifested by the large angle observed between the two corresponding vectors (given by means of their correlation $\zeta_{H_I^{(2b)},H_I^{tot}}$). In fact, the heavier the nucleus to be considered, the larger the deviation. E.g., for a six-nucleon ($A = 6$) system, the H_I^{tot} vector gives the total induced interaction for the SRG$^{a=6}$, and $H_I^{(2b)}$ vector gives the total SRG$^{a=2}$-induced interaction propagated to $A = 6$. Clearly, both vectors possess a comparatively small similarity with a correlation coefficient, $\zeta_{H_I^{(2b)},H_I^{tot}} = .45$ (or 63-degree angle between the corresponding vectors) for both N^{3}LO and JISP16. The square of the correlation coefficient, $\zeta^2_{H_I^{(2b)},H_I^{tot}}$, indicates the portion of the H_I^{tot} that behaves as the $H_I^{(2b)}$ interaction (Fig. 4). That is, this portion of H_I^{tot} yields the same energy spectrum for an A-particle system as the one produced by the $H_I^{(2b)}$ for the same number of particles. Likewise, $1 - \zeta^2_{H_I^{(2b)},H_I^{tot}}$ demonstrates the contribution of interactions in H_I^{tot} not accounted for by $H_I^{(2b)}$ but needed to retain the SRG unitarity in a general many-body system. Indeed, the results indicate that these interactions make up a considerable fraction of the

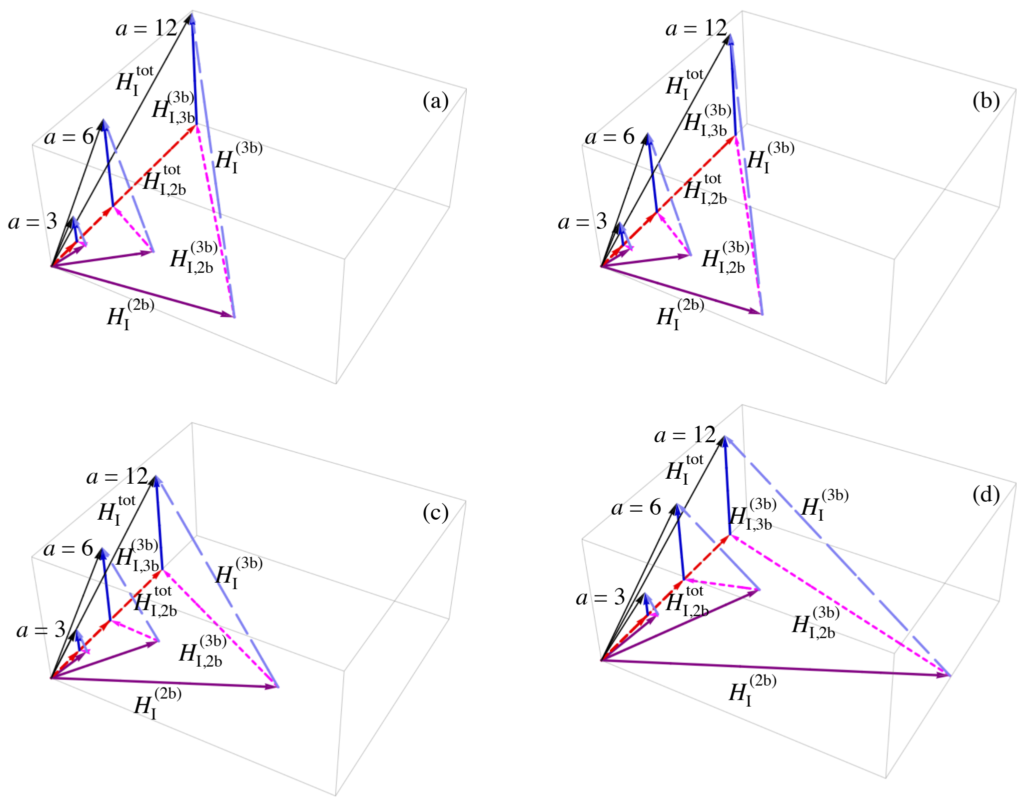

FIG. 3: (Color online) Vector representation of the SRG-induced interactions (Table I) relative to the NN interaction strength. In the horizontal plane: $H_I^{(2b)}$ (purple, solid), $H_{I,2b}^{(3b)}$ (magenta, dotted), and total $H_{I,2b}^{tot}$ (red, dashed); in the vertical plane: pure 3-body $H_{I,3b}^{(3b)}$ (blue, along the vertical axis) and total H_I^{tot} (black); and $H_I^{(3b)}$ (light blue, long dashed). Induced interactions are shown for (a) N^{3}LO, (b) JISP16, (c) CD-Bonn, and (d) AV18 NN interactions and for 6-level $a = 3$ (smallest set of vectors), 6, and 12 (largest set of vectors) model spaces. For each a, the vector corresponding to the $H_{I,2b}^{tot}$ is fixed along the y-axis.

total induced interaction. E.g., as shown in Fig. 4, while the $H_I^{(2b)}$-like portion of H_I^{tot} is comparatively large for $A = 3$ $(50 - 90\%)$, it rapidly decreases for heavier nuclei and becomes almost negligible in heavier systems. The outcome holds for both 6-level and 10-level model spaces, as seen in Fig. 4. This, in turn, has a direct consequence on the applicability of an SRG$^{a=2}$ renormalized interaction to light nuclei. Namely, without the important $H_{I,2b}^{(3b)}$, the unitarity for SRG$^{a=2}$-evolved interactions no longer holds for $A > 3$ nuclei and hence, when employed in nuclear structure and reaction calculations, may describe only certain spectral features.

While it is clear that SRG evolving H_{NN} with a 1-body C yields a renormalized interaction that appears to be 2-body driven, the SRG, if restricted to an $a = 2$ system, neglects a large 3-body contribution and hence is not suitable for $A \geq 3$ nuclear structure applications. An SRG$^{a=3}$ neglects, in addition to an even smaller contribution of higher particle rank interactions, induced 4-body interactions. For reasonable λ_d, the only significant contribution of the latter emerges through their up-to-3-body part, in particular, through their projection along the $[\eta_0, H_0]$ interaction. This, as mentioned above, only affects the overall strength of the total induced interaction. Note that the most dominant induced contribution is 5-body if evolving H_{NN+3N}, which requires at least SRG$^{a=5}$ calculations. This term is 4-body for evolving H_{NN} with the 2-body C_2^{su3}, the second-order Casimir invariant of SU(3), or the 2-body $T_{\rm rel}$ relative kinetic energy. Fortunately, in the SU(3) case, the use of symmetry renders 4-body terms manageable.

Finally, it is interesting to point out that the overall behavior of both N^{3}LO and JISP16 is essentially similar in the model spaces considered. Indeed, while other interactions manifest various differences, the properties studied here for both N^{3}LO and JISP16 interactions reveal a considerable similarity (see, Fig. 1, Fig. 3 (a) and (b), as well as Fig. 4, red filled diamonds and green squares).

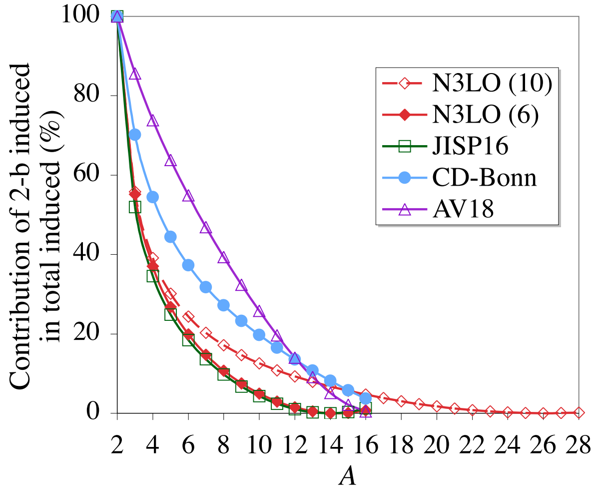

FIG. 4: (Color online) Portion of the total SRG-induced interaction H_I^{tot} that yields the same energy spectrum for an A-particle system as the one produced by the 2-body SRG-induced $H_I^{(2b)}$ interaction in the same A-particle system for various NN realistic interactions, $\mathrm{N^3LO}$ (for 10 and 6 levels), as well as JISP16, CD-Bonn, and AV18 (6 levels).

V. CONCLUSIONS

In the SDT framework, we applied the SRG renormalization approach to various NN realistic interactions and, for the first time, investigated the overall contribution of the SRG-induced many-body interactions and their effective 2-body part for many-nucleon systems, up through $A = 28$ particles. This was done by allowing the nucleons to interact through the most dominant SRG-induced interaction of the $[\eta_0, H_0]$ kind, which in the present case is up-to-3-body (leaving out only negligible contributions of higher-order interactions). The size of various contributions was estimated by their second-order energy moment (strength σ). For A particles, these strengths were evaluated with the help of SDT using only the 3-particle information. We note that the procedure yields exactly the same strengths as if one were to construct the corresponding many-body Hamiltonians for A particles and then calculate their norm. Results are shown for SRG flows not infinitely evolved and using the free HO Hamiltonian $C = H_{\mathrm{HO}}$ (one-body) for $\mathrm{N^3LO}$ and JISP16, as well as, for illustration, CD-Bonn and AV18 realistic NN interactions in m-scheme basis for six to ten j-levels up through the pf-shell and for like particles.

Among the many-body SRG-induced interactions, necessary to ensure the unitarity of SRG transformations, only those that emerge at the very beginning of the SRG transformations play a key role and above all, have a low particle rank. What we find here is that, for a 1-body C and a 2-body initial Hamiltonian, 3-body interactions are crucial. Nonetheless, their major contribution is found to be 2-body rendering a simpler final SRG-evolved Hamiltonian. This remarkable result reveals that the SRG-renormalized interaction is essentially two-body driven. While it is clear that 3-body interactions need to be taken into account, for certain problems, retaining only the 2-body part of the SRG-evolved many-body Hamiltonian may be sufficient. Above all, the extraction of this 2-body part is readily available in the SDT framework. This reduces the nuclear eigenvalue problem to one that employs manageable basis spaces with simple one-body and two-body inter-nucleon interactions.

The significance of the 3-body induced interaction, in turn, has a direct consequence on the applicability of an $\mathrm{SRG}^{a=2}$ renormalized interaction to light nuclei. Namely, without the important two-body part of the 3-body term, $\mathrm{SRG}^{a=2}$-evolved interactions are no longer unitarily equivalent to the original NN interaction for $A > 3$ nuclei and hence, when employed in nuclear structure and reaction calculations, may describe only certain spectral features. If a realistic $NN + 3N$ interaction is employed, the initial dominating SRG-induced term is up to 5-body and requires SDT propagation formulae for interactions of a particle rank ≤ 5. The SDT-based method used in the present study can also be applied to other choices for the SRG-generating operator (C) and NN interactions, as well as to $3N$ interactions.

In short, we carried forward first studies of the overall many-body contributions to an SRG-evolved interaction in a many-particle system at an operator level (based on properties of the Hamiltonian) without restricting to energy spectra observations, and found that 3-body interactions and their 2-body part play a significant role.

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Appendix A: Derivation of pure ν-body interactions

We follow [12] to derive the pure 0-, 1-, 2-, and 3-body interactions of a 3-body interaction like $H_I^{(3b)}$ of Eq. (2). For a scalar partitioning of the HO basis space of dimension $\mathcal{N}$, the definite particle rank (pure ν-body) interactions, $\mathcal{H}^{(k)}(\nu)$, for a given k-body Hamiltonian $H(k)$ and A particles are given as,

$$\mathcal{H}^{(k)}(\nu) = \frac{1}{(k-\nu)!\binom{\mathcal{N}-2\nu}{k-\nu}} \sum_{t=k-\nu}^{k} \frac{(-)^{t-k+\nu}}{(t-k+\nu)!} \binom{\mathcal{N}-\nu-k+t+1}{t-k+\nu}^{-1} \binom{A-k+t}{t-k+\nu} D^t H(k). \quad \text{(A1)}$$

In (A1), the $D^tH(k)$ unitary-scalar contractions of an operator H are defined as,

$$D^tH(k) = \sum_i \left\{ a_i^\dagger, [a_i, D^{t-1}H(k)] \right\}, \quad \text{(A2)}$$

and $D^0H(k) \equiv H(k)$. Here, $\{\mathcal{A},\mathcal{B}\}$ and $[\mathcal{A},\mathcal{B}]$ denote anti-commutator and commutator, respectively. Hence, a 3-body interaction ($k = 3$),

$$H(3) = \frac{1}{(3!)^2} \sum_{ijqrsk} W_{ijqrsk} a_i^\dagger a_j^\dagger a_q^\dagger a_k a_s a_r, \quad \text{(A3)}$$

can be expanded into interactions of a definite particle rank using (8),

$$\begin{aligned} H(3) &= \binom{A}{3}\mathcal{H}^{(3)}(0) + \binom{A-1}{2}\mathcal{H}^{(3)}(1) \\ &+ (A-2)\mathcal{H}^{(3)}(2) + \mathcal{H}^{(3)}(3), \end{aligned} \quad \text{(A4)}$$

where, according to (A1) with $k = 3$,

$$\begin{aligned} \mathcal{H}^{(3)}(0) &= \frac{1}{3!}\frac{1}{\binom{\mathcal{N}}{3}} D^3H(3) \equiv W_c^{(3)}, \\ \mathcal{H}^{(3)}(1) &= \frac{1}{2!}\frac{1}{\binom{\mathcal{N}-2}{2}} \left(D^2H(3) - \frac{A}{\mathcal{N}} D^3H(3) \right), \\ \mathcal{H}^{(3)}(2) &= \frac{1}{\mathcal{N}-4} \left(DH(3) - \frac{A-1}{\mathcal{N}-2} D^2H(3) \right. \\ &\left. + \frac{1}{2}\frac{\binom{A}{2}}{\binom{\mathcal{N}-1}{2}} D^3H(3) \right), \\ \mathcal{H}^{(3)}(3) &= H(3) - \frac{A-2}{\mathcal{N}-4} DH(3) + \frac{1}{2}\frac{\binom{A-1}{2}}{\binom{\mathcal{N}-3}{2}} D^2H(3) \\ &- \frac{1}{3!}\frac{\binom{A}{3}}{\binom{\mathcal{N}-2}{3}} D^3H(3). \end{aligned} \quad \text{(A5)}$$

The D-interactions are derived with the help of (A2),

$$\begin{aligned} D^3H(3) &= \left(\sum_{ijq} W_{ijqijq} \right), \\ D^2H(3) &= \sum_{ir} \left(\sum_{jq} W_{ijqrjq} \right) a_i^\dagger a_r, \\ DH(3) &= \frac{1}{4} \sum_{ijrs} \left(\sum_q W_{ijqrsq} \right) a_i^\dagger a_j^\dagger a_s a_r. \end{aligned} \quad \text{(A6)}$$

Hence, the first term in each $\mathcal{H}^{(3)}(\nu)$ of Eqs. (A5) gives Eqs. 15, 16, and 18. The traceless counterparts are obtained by considering the remaining terms in (A5), which yields Eqs. 17 and 19.

[1] S. D. Glazek and K. G. Wilson, Phys. Rev. D **48**, 5863 (1993); Phys. Rev. D **49**, 4214 (1994).
[2] F. Wegner, Ann. Phys. (Leipzig) **3**, 77 (1994).
[3] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, Phys. Rev. C **75**, 061001 (2007).
[4] R. Roth, S. Reinhardt, and H. Hergert, Phys. Rev. C **77**, 064003 (2008).
[5] P. Navrátil, J. P. Vary, and B. R. Barrett, Phys. Rev. Lett. **84**, 5728 (2000); Phys. Rev. C **62**, 054311 (2000).
[6] M. Wloch *et al.*, Phys. Rev. Lett. **94**, 212501 (2005).
[7] T. Dytrych *et al.*, Phys. Rev. Lett. **98**, 162503 (2007).
[8] P. Navrátil *et al.*, J. Phys. G: Nucl. Part. **36**, 083101 (2009); R. Roth and P. Navrátil, Phys. Rev. Lett. **99**, 092501 (2007).
[9] K.D. Launey, T. Dytrych, J. P. Draayer, and G. Popa, J. Phys. A: Math. Theor. **45**, 015208 (2012).
[10] J. B. French, Phys. Lett. **23**, 248 (1966).
[11] J. B. French and K. F. Ratcliff, Phys. Rev. C **3**, 94 (1971).
[12] F. S. Chang, J. B. French, and T. H. Thio, Ann. Phys. (N.Y.) **66**, 137 (1971).
[13] V. K. B. Kota and R. U. Haq, "Spectral Distributions in Nuclei and Statistical Spectroscopy," (World Scientific Publishing Co., 2010).
[14] A. F. Lisetskiy, M. K. G. Kruse, B. R. Barrett, P. Navratil, I. Stetcu, and J. P. Vary, Phys. Rev. C **80**, 024315 (2009).
[15] G. Hagen *et al.*, Phys. Rev. C **76**, 034302 (2007).
[16] K. Tsukiyama, S. K. Bogner, and A. Schwenk, Phys. Rev. Lett. **106**, 222502 (2011).
[17] K. T. Hecht and J. P. Draayer, Nucl. Phys. A **223**, 285 (1974).
[18] K. F. Ratcliff, Phys. Rev. C **3**, 117 (1971).
[19] J. N. Ginnochio, Phys. Rev. Lett. **31**, 1260 1973
[20] J. P. Draayer, J. B. French, M. Prasad, V. Potbhare, and S. S. M. Wong, Phys. Lett. **57B**, 130 (1975).
[21] J. B. French and V. K. B. Kota, Phys. Rev. Lett. **51**, 2183 (1983).
[22] B. Strohmaier, S. M. Grimes and H. Satyanarayana, Phys. Rev. C **36**, 1604 (1987).
[23] A. Abzouzi, E. Caurier, and A. P. Zuker, Phys. Rev. Lett.

66, 1134 (1991).
[24] T. R. Halemane, K. Kar, and J. P. Draayer, Nucl. Phys. A **311**, 301 (1978).
[25] B. J. Dalton, W. J. Baldridge, and J. P. Vary, Phys. Rev. C **20**, 1908 (1979).
[26] L. Benet, T. Rupp, and H. A. Weidenmiiller, Phys. Rev. Lett. **87**, 010601 (2001).
[27] S. Tomsovic, M. B. Johnson, A. Hayes, and J. D. Bowman, Phys. Rev. C **62**, 054607 (2000).
[28] M. Horoi, M. Ghita, and V. Zelevinsky, Phys. Rev. C **69**, 041307(R) (2004).
[29] Y. M. Zhao, A. Arima, N. Yoshida, K. Ogawa, N. Yoshinaga, and V. K. B. Kota, Phys. Rev. C **72**, 064314 (2005).
[30] K. D. Sviratcheva, J. P. Draayer, and J. P. Vary, Nucl. Phys. A **786**, 31 (2007).
[31] E. D. Jurgenson, P. Navrátil, and R. J. Furnstahl, Phys. Rev. Lett. **103**, 082501 (2009).
[32] R. Roth, J. Langhammer, A. Calci, S. Binder, and P. Navrátil, Phys. Rev. Lett. **107**, 072501 (2011).
[33] D. R. Entem and R. Machleidt, Phys. Rev. C **68**, 041001 (2003).
[34] A. M. Shirokov *et al.*, Phys. Letts. B **644**, 33 (2007).
[35] R. Machleidt, Phys. Rev. C **63**, 024001 (2001).
[36] R.B. Wiringa, V.G.J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).