

Unmixing Symmetries

Calvin W. Johnson *Department of Physics, San Diego State University, 5500 Campanile Drive, San Diego, California 02182-1233, USA*

(Received 3 December 2019; revised manuscript received 18 February 2020; accepted 20 April 2020; published 29 April 2020)

The low-lying spectra of atomic nuclei display diverse behaviors, for example, rotational bands, which can be described phenomenologically by simple symmetry groups such as spatial $SU(3)$. This leads to the idea of dynamical symmetry, where the Hamiltonian commutes with the Casimir operator(s) of a group, and is block diagonal in subspaces defined by the group's irreducible representations or irreps. Detailed microscopic calculations, however, show these symmetries are in fact often strongly mixed and the wave function fragmented across many irreps. More commonly, the fragmentation across members of a band are similar, which is called a quasidynamical symmetry. In this Letter I explicitly, albeit numerically, construct unitary transformations from a quasidynamical symmetry to a dynamical symmetry, adapting the similarity renormalization group (SRG) in order to transform away the symmetry-mixing parts of the Hamiltonian. The standard SRG produces unsatisfactory results, forcing the induced dynamical symmetry to be dominated by high-weight irreps irrespective of the original decomposition. Using spectral distribution theory to rederive and diagnose standard SRG, I introduce a new form of SRG. The new SRG transforms a quasidynamical symmetry to a dynamical symmetry, that is, unmixes the mixed symmetries, with intuitively more appealing results.

DOI: [10.1103/PhysRevLett.124.172502](https://doi.org/10.1103/PhysRevLett.124.172502)

The spectra of atomic nuclei display a rich portfolio of behaviors, the most striking of which are rotational and vibrational bands. These can be elegantly described using spectrum-generating algebras whose eigenspectra as well as transition probabilities (up to an overall scale) capture experimental data. This leads to the idea of a *dynamical symmetry* [1,2], marked by the Hamiltonian commuting with the group's Casimir operator and the wave functions wholly contained within a single irreducible representation (irrep) of the underlying group. Dynamical symmetries of this kind are mostly invoked in nuclear structure physics, with some discussions in atomic and molecular physics [3–7].

The problem is, microscopic calculations showing true dynamical symmetries are rare. Standard pieces of the nuclear force, such as spin-orbit splitting and pairing [8–11], strongly break the symmetry and mix irreps. This is puzzling in light of the fact that one can empirically use algebraic methods to reproduce data. A further piece of the puzzle is the existence of *quasidynamical symmetries* [12–14], where the pattern of mixing symmetries, although often very complex, is similar across members of a band.

In this Letter I adapt a method, the similarity renormalization group (SRG), to generate a unitary transformation that largely *unmixes* the symmetry. (I use “mixing” rather than “breaking” symmetry because the former better matches the continuous process described below.) The standard SRG, however, produces for some states unsatisfactory results, so I introduce a novel variant of SRG which provides more intuitively appealing results. Thus I can transform away the symmetry-mixing terms in a

Hamiltonian. As a bonus, a new light is shed on the behavior of SRG, a widely used method.

To illustrate the mixing of symmetries I decompose nuclear wave functions, calculated via configuration-interaction, into subspaces defined by irreducible representations. Let $\hat{C}$ be a Casimir operator for a group, and let z denote eigenvalues of the Casimir, so that $\hat{C}|z, \alpha\rangle = z|z, \alpha\rangle$. The eigenvalues are highly degenerate and can label subspaces or irreducible representations. An familiar example is the rotation group, with the Casimir $\hat{J}^2$ with eigenvalues $j(j+1)$ labeling subspaces of good total angular momentum. For a given state $|\Psi\rangle$, define the fraction of the wave function in a subspace labeled by z as

$$f(z) = \sum_{\alpha} |\langle z, \alpha | \Psi \rangle|^2. \quad (1)$$

For dynamical symmetries, $f(z) = 1$ for some value of z , and zero for all other values. For any state, however, one can calculate $f(z)$ efficiently [11,15,16].

Figure 1 shows calculations of ^{36}Ar in the $1s_{1/2} - 0d_{3/2} - 0d_{5/2}$ or *sd* shell, which has a frozen ^{16}O core, using the phenomenological universal *sd* interaction version “B” (USDB) [17], which I decomposed using the quadratic $SU(3)$ Casimir, $\hat{C}_2 = \vec{Q} \cdot \vec{Q} + 3L^2$, where L is orbital angular momentum and $\vec{Q}$ is the so-called Elliott quadrupole operator. The eigenvalues of $\hat{C}_2$ can be expressed in terms of integer quantum numbers λ and μ , $4(\lambda^2 + \lambda\mu + \mu^2 + 3\lambda + 3\mu)$ [1]. Because I use only one of

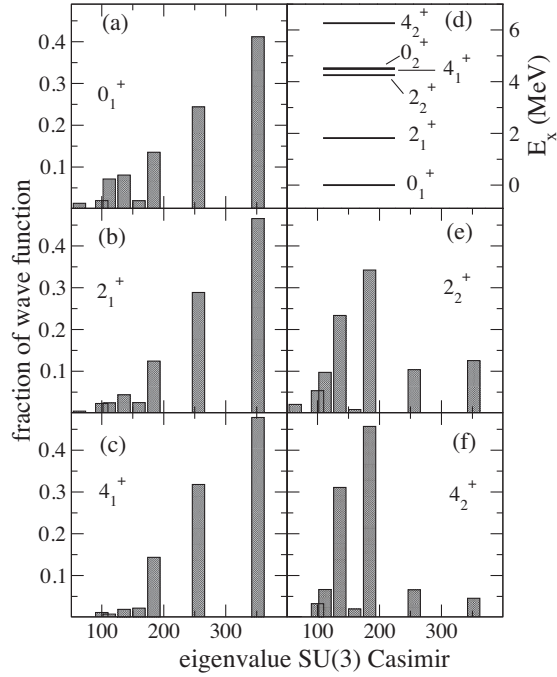


FIG. 1. Low-lying levels and SU(3) decompositions for ^{36}Ar in the sd shell using the USDB interaction. Panels (a)–(c) show the ground state band, while panels (e) and (f) show the excited γ band. Panel (d) shows the calculated excitation energies.

two SU(3) Casimirs, the decompositions are in many cases sums of irreps. One can interpret the results in terms of (λ, μ) of SU(3), but I leave those off precisely because those details, while of interest to the specialist, are irrelevant to the points being made here. I chose ^{36}Ar because it is tractable for the following calculations, has strong mixing, yet clearly demonstrates a quasidynamical symmetry. Other nuclides show similar results.

Note that the pattern of fragmentation of the wave function over irreps is repeated across several states [8,11]. This is an example of quasidynamical symmetry, which turns out to be surprisingly commonplace.

Seeing the repeated patterns of quasidynamical symmetries, it is natural to wonder if one could transform away the symmetry-mixing terms to regain a true dynamical symmetry. While it is not yet known how to choose analytically such a unitary transformation, there does exist a well-known method for numerically constructing unitary transformations, the similarity renormalization group [18–24]. SRG is widely used in nuclear physics to soften nuclear forces for *ab initio* calculations, by approximately decoupling low-momentum and high-momentum states, with analogous applications in atomic and molecular physics [25], nonrelativistic reduction of the Dirac equation [26], and particle physics [27]. In each case one uses SRG to approximately decouple a model space from the rest of the space to improve convergence of calculations. Here I present a novel use of SRG to decouple or unmix group symmetries. The beauty of this approach is

that it does not require explicit knowledge of the origin of symmetry mixing.

Consider a parametrized unitary transformation of a Hamiltonian, $\hat{H}(s) = \hat{U}(s)\hat{H}\hat{U}^\dagger(s)$, and let $\hat{\eta} = (d\hat{U}(s)/ds)\hat{U}^\dagger(s)$ be an anti-Hermitian operator. Then one can construct an equation for unitary evolution,

$$\frac{d\hat{H}(s)}{ds} = [\hat{\eta}, \hat{H}(s)]. \quad (2)$$

For standard SRG, one introduces a fixed Hermitian operator called the *generator*, $\hat{G}$, and then choose

$$\hat{\eta} = [\hat{G}, \hat{H}(s)]. \quad (3)$$

To soften the nuclear interaction, one typically uses the kinetic energy operator $\hat{T}$ as the generator; there are other generators for other applications, such as the in-medium SRG [23,24]. Instead, here I chose $\hat{G}$ to be $-\hat{C}_2$ of SU(3) (the minus sign is because one knows [28] that $-\vec{Q} \cdot \vec{Q}$ is an approximate component of the nuclear force), although in principle one could use any group Casimir. In order to ensure exact unitarity, I act directly on the many-body matrix, which here is of dimension 640; thus the energy spectrum is unchanged, which was confirmed after evolution. The differential equation is solved using fourth-order Runge-Kutta. (There are more sophisticated methods for solving SRG [29], but Runge-Kutta is straightforward to code.) Because the SU(3) Casimir has no meaningful dimensions, I rescaled $\hat{\eta}$ so that the two-norm $\|\hat{\eta}\| = 1$, and the evolution parameter s is dimensionless.

Figure 2 shows decompositions for two states, the 0_1^+ ground state and the 2_2^+ state, as the Hamiltonian is evolved under SRG, starting at $s = 0$ along the top row, and then increasing to $s = 2$ along the bottom row. While the Hamiltonian is evolved, the decomposition was performed using the original SU(3) Casimir. The left-hand column shows the evolution for the 0_1^+ ground state under the “standard” SRG, which uses Eq. (3), while the middle column shows the same for the 2_2^+ state. In both cases the decomposition evolves to a single irrep, that is, dynamical symmetry.

Yet upon closer inspection, something goes “wrong” under SRG evolution. While the ground state essentially has all its strength going into the irrep which already has the largest fraction, as one might expect or at least hope for, the 2_2^+ state goes to a higher-weight irrep barely occupied in the original decomposition.

Why does SRG drive the fractional distribution to the “wrong” irreps? To understand this, I borrow concepts from spectral distribution theory [30–32]. A key idea in spectral distribution theory is the introduction of an inner product on a linear space of Hermitian operators, represented by finite Hermitian matrices with dimension N . For two such operators, $\mathbf{A}$, $\mathbf{B}$ (from here on I use boldface type to emphasize they are finite matrices), the inner product is

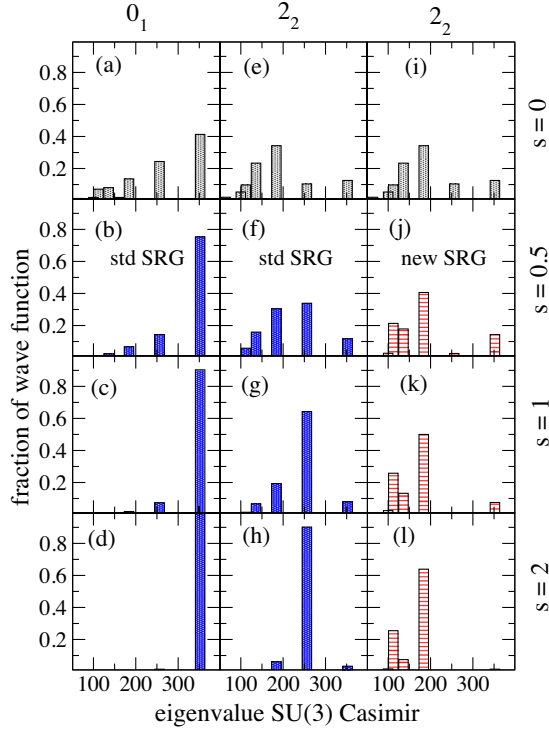


FIG. 2. Decomposition of the 0_1^+ and 2_2^+ states of ^{36}Ar , using original ($s = 0$) and SRG-evolved ($s > 0$) Hamiltonians. Here s is dimensionless. The top row, (a), (e), and (i), gives the decompositions for states from unevolved Hamiltonians. The left-hand column, (a)–(d), shows the evolution under the standard SRG for the 0_1^+ state. The middle column, (e)–(h), shows the evolution under standard SRG for the 2_2^+ states, while the right-hand column, (i)–(l), shows the evolution under the new SRG for the 2_2^+ state. Not shown is the evolution of the 0_1^+ state under the new SRG, which is nearly indistinguishable to the evolution under standard SRG.

$$(A, B) = \frac{1}{N} \text{tr} \mathbf{A} \mathbf{B} - \frac{1}{N} \text{tr} \mathbf{A} \frac{1}{N} \text{tr} \mathbf{B}. \quad (4)$$

With an inner product one can define how close or different two Hermitian operators are, and even define an “angle” between two interactions.

Now suppose we want a unitary transformation on a Hamiltonian $\mathbf{H}$ that makes it as close as possible to the generator $\mathbf{G}$. Because N is fixed, $\mathbf{G}$ is fixed, and, by unitarity, $\text{tr} \mathbf{H}$ is fixed; this means we want to maximize $\text{tr} \mathbf{G} \mathbf{H}(s)$. While guaranteeing a global maximum is not trivial, let us suppose we follow the generic evolution Eq. (2) and choose to maximize the *rate* at which the unitary transformation increases $\text{tr} \mathbf{G} \mathbf{H}(s)$; that is, we want to maximize

$$\frac{d}{ds} \text{tr} \mathbf{G} \mathbf{H}(s) = \text{tr} \mathbf{G} \frac{d}{ds} \mathbf{H}(s) = \text{tr} \mathbf{G} [\eta, \mathbf{H}(s)], \quad (5)$$

where I used Eq. (2) to replace the derivative. Using the cyclic property of traces, $\text{tr} \mathbf{A} \mathbf{B} = \text{tr} \mathbf{B} \mathbf{A}$, one can rewrite the right-hand side of Eq. (5):

$$\begin{aligned} \text{tr} \mathbf{G} [\eta, \mathbf{H}(s)] &= \text{tr} \mathbf{G} \eta \mathbf{H}(s) - \text{tr} \mathbf{G} \mathbf{H}(s) \eta \\ &= \text{tr} \eta \mathbf{H}(s) \mathbf{G} - \text{tr} \eta \mathbf{G} \mathbf{H}(s) = \text{tr} \eta [\mathbf{H}(s), \mathbf{G}], \end{aligned} \quad (6)$$

which is maximized when the antisymmetric matrix $\eta = [\mathbf{H}(s), \mathbf{G}]^T = [\mathbf{G}, \mathbf{H}(s)]$. Standard SRG is defined by maximizing the rate $\mathbf{H}(s)$ approaches the generator $\mathbf{G}$, forcing $\mathbf{H}(s)$ to be as similar as possible to $\mathbf{G}$.

This explains the behavior of mixed symmetries under standard SRG: by forcing $\mathbf{H}$ to be as similar as possible to the $\text{SU}(3)$ Casimir $-\mathbf{C}_2$, standard SRG tries to match extremal eigenpairs: low-lying states of $\mathbf{H}$ are driven to be like high-weight states of the Casimir.

I now present an alternative. Recall that a dynamical symmetry is when a Hamiltonian merely *commutes* with the Casimir(s) of a group. Thus, for my purposes here, a more appropriate condition is to maximize $\text{tr} [\mathbf{G}, \mathbf{H}(s)]^\dagger [\mathbf{G}, \mathbf{H}(s)]$, or, more practically, choose the evolution equation that maximizes its decrease. Following the same methodology as before, one arrives at a modified SRG procedure, with

$$\hat{\eta} = [[[\mathbf{G}, \mathbf{H}(s)], \mathbf{H}(s)], \mathbf{G}]. \quad (7)$$

Properly coded, this only takes twice as much time as the original SRG. The right-hand column of Fig. 2 shows the decomposition of the 2_2^+ state under this “new” SRG. Now the strength is pushed to irreps already in the plurality in the original decomposition. (The decomposition of the 0_1^+ state under both SRGs is nearly indistinguishable).

These results are not unique. Figure 3 shows the decomposition for the six lowest states, using both SRG equations, evolved to $s = 3$. For the ground state band (left-hand column, the 0_1^+ , 2_1^+ , 4_1^+ states), the decompositions are indistinguishable and I show only the results from standard SRG. For the 0_2^+ , 2_2^+ , 4_2^+ states, there is a difference, with standard SRG leading to the wave function being predominant in a higher-weight (and, compared to decomposition of states from the unevolved Hamiltonian, wrong) irrep, while the decomposition for states from the new SRG better reflect the unevolved state. Note that under the new SRG a secondary component persists; evolving further to $s = 5$, the results are little changed.

More insight about the evolution can be gleaned from Fig. 4. Using the inner product (4), one can calculate the angle between any two Hamiltonian-like operators. Figure 4(a) shows the angle between the generator $\mathbf{G}$ [here $-\mathbf{C}_2$, the $\text{SU}(3)$ Casimir] and the evolved Hamiltonian $\mathbf{H}(s)$, while Fig. 4(b) shows the angle between the evolved Hamiltonian and the original $\mathbf{H}(0)$, with solid black lines for the standard SRG and dashed (red) lines for the new SRG. In both measurements, the new SRG evolves the Hamiltonian “less far away” than standard SRG.

This is confirmed in Table I, which gives the numerical overlap between the wave functions from the unevolved Hamiltonian, and Hamiltonians evolved by the standard

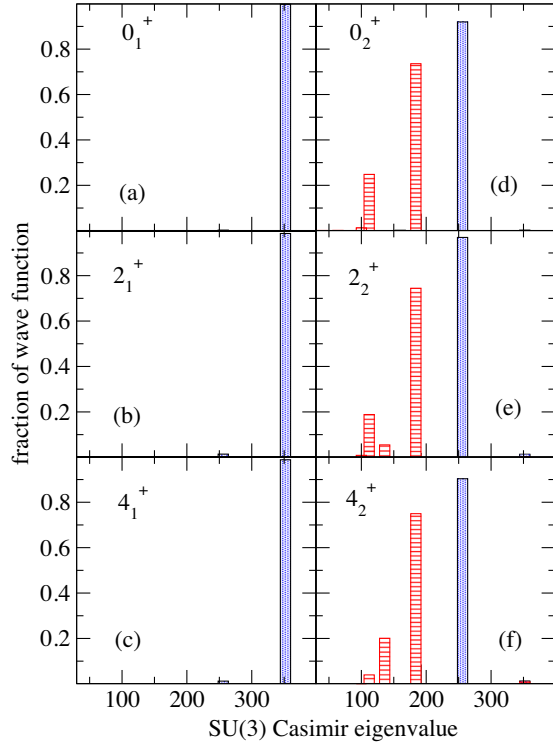


FIG. 3. SU(3) decompositions for low-lying levels ^{36}Ar in the sd shell using the USDB interaction, evolved under two different SRG equations to $s = 3$. Solid (blue) bars are for standard SRG, while (red) horizontal strips are for the new SRG. For the ground state band, that is, the 0_1^+ , 2_1^+ , 4_1^+ states, the two evolutions are indistinguishable.

and new SRG out to $s = 3$. It confirms that the ground state band, which is dominated by the highest weight irrep, has nearly identical evolution under both SRGs, but that for the 0_2^+ , 2_2^+ , 4_2^+ states, the new SRG leads to states with a much larger overlap with the unevolved states than standard SRG.

Because the motivation of the new SRG was to reduce the commutator $[\mathbf{H}(s), \mathbf{G}]$, Fig. 4(c) shows the magnitude of the commutator, normalized to 1 at $s = 0$. The magnitude is computed using the two-norm, but because the commutator is an antisymmetric matrix, this is the same as Eq. (4) up to a minus sign. The commutator for the new SRG indeed drops more rapidly at first, although for large s the standard SRG overtakes it.

It is well known that SRG induces many-body forces even when starting from purely two-body interactions. In my evolution I worked directly with the many-body Hamiltonian. Nonetheless, I estimated the amount of induced many-body forces. At $s = 0$, most of the matrix elements of $\mathbf{H}$ are in fact zero, due to the two-body nature of the Hamiltonian. For $s > 0$, I measured what fraction of $\text{tr}\mathbf{H}^2$ came from those matrix elements that were originally zero. Shown in Fig. 4(d), this at the very least gives a lower limit on the induced many-body interactions. Unsurprisingly given the triple commutator of Eq. (7), the

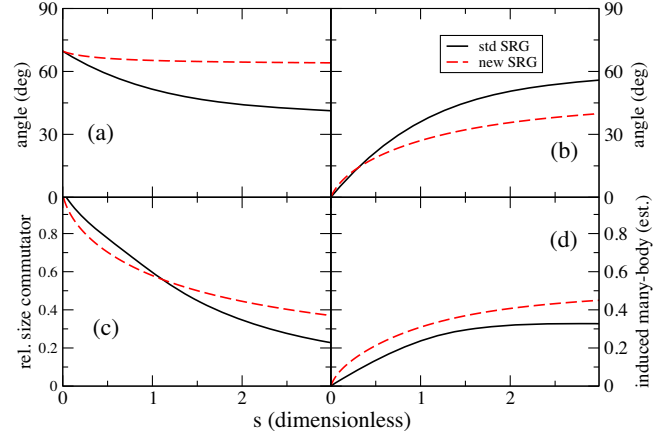


FIG. 4. Tracking the evolution as a function of s of the Hamiltonian for ^{36}Ar , with solid (black) line for standard SRG and dashed (red) line for the new SRG. (a) Angle, as defined by spectral distribution theory (see text for details), between evolved $\hat{H}(s)$ and the generator $\mathbf{G}$, here the quadratic SU(3) Casimir. (b) Angle between evolved $\mathbf{H}(s)$ and original Hamiltonian $\mathbf{H}(0)$. (c) Magnitude of the commutator $[\mathbf{H}(s), \mathbf{G}]^2$, relative to magnitude at $s = 0$. (d) Estimated fraction of $\hat{H}(s)$ with induced many-body terms.

new SRG induces a larger fraction of many-body components, but still of comparable size to the standard SRG. In practical applications one will likely have to either include the induced three-body terms [21] or carry out some effective procedure such as in-medium SRG, where one normal orders three-body and higher-order terms with respect to a reference state [23,24]. Because such procedures work well with standard SRG, there is no reason to think it will be different here.

Although I only show the case of ^{36}Ar , other nuclides show similar behavior. When the decomposition is highly fragmented and the wave function from the unevolved Hamiltonian is not dominated by a single irrep, both SRG procedures will still drive the decomposition to a single irrep: the original SRG will still evolve to a high-weight irrep, even if that irrep had a small occupation originally, while under the new SRG the evolved dominant irrep tends to be near the average of the previously occupied irreps. The implications of this behavior will be investigated in future work.

TABLE I. Overlaps between configuration-interaction wave functions, calculated using the unevolved ($s = 0$) Hamiltonian and evolved to $s = 3$ using the standard and new SRG.

	0_1^+	2_1^+	4_1^+	0_2^+	2_2^+	4_2^+
$\langle \psi(s=0) \psi_{\text{std}}(s=3) \rangle$	0.669	0.719	0.717	0.008	0.336	0.382
$\langle \psi(s=0) \psi_{\text{new}}(s=3) \rangle$	0.643	0.696	0.702	0.561	0.695	0.836
$\langle \psi_{\text{std}}(s=3) \psi_{\text{new}}(s=3) \rangle$	0.999	0.992	0.991	0.007	0.201	0.170

In summary, I have shown how to construct a unitary transformation that undoes mixed symmetries, by transforming away symmetry-mixing terms, leading to a system with nearly pure dynamical symmetry. Furthermore, I introduced and demonstrated a new version of SRG that, at least in some aspects, provides superior behavior over standard SRG. One possible application beyond “unmixing” symmetries would be in *symmetry-adapted* structure calculations [33], which rely upon the wave functions being dominated by a few irreps; by reducing the fragmentation into other irreps, such calculations could be closer to the full-space results. Because this new SRG decouples differently from, and in some cases demonstrably better than standard SRG, it may have applications beyond unmixing symmetries.

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics, under Award No. DE-FG02-96ER40985.

-
- [1] I. Talmi, *Simple Models of Complex Nuclei* (Harwood Academic Publishers, Chur, 1993).
 - [2] D. J. Rowe and J. L. Wood, *Fundamentals of Nuclear Models: Foundational Models* (World Scientific, Singapore, 2010).
 - [3] C. Wulfman, *Chem. Phys. Lett.* **23**, 370 (1973).
 - [4] D. R. Herrick and M. E. Kellman, *Phys. Rev. A* **18**, 1770 (1978).
 - [5] F. Iachello and R. D. Levine, *Algebraic Theory of Molecules* (Oxford University Press, Oxford, 1995).
 - [6] L. Cederbaum, *J. Chem. Phys.* **103**, 562 (1995).
 - [7] D. Baykusheva, M. S. Ahsan, N. Lin, and H. J. Wörner, *Phys. Rev. Lett.* **116**, 123001 (2016).
 - [8] P. Rochford and D. Rowe, *Phys. Lett. B* **210**, 5 (1988).
 - [9] C. Bahri, J. Escher, and J. Draayer, *Nucl. Phys. A* **592**, 171 (1995).
 - [10] J. Escher, C. Bahri, D. Troltenier, and J. Draayer, *Nucl. Phys. A* **633**, 662 (1998).
 - [11] V. G. Gueorguiev, J. P. Draayer, and C. W. Johnson, *Phys. Rev. C* **63**, 014318 (2000).
 - [12] C. Bahri, D. J. Rowe, and W. Wijesundera, *Phys. Rev. C* **58**, 1539 (1998).
 - [13] D. J. Rowe, in *The Nucleus: New Physics for the New Millennium*, edited by F. D. Smit, R. Lindsay, and S. V. Försch (Springer Science and Business Media, New York, 2000), pp. 379–395.
 - [14] C. Bahri and D. Rowe, *Nucl. Phys. A* **662**, 125 (2000).
 - [15] C. W. Johnson, *Phys. Rev. C* **91**, 034313 (2015).
 - [16] R. A. Herrera and C. W. Johnson, *Phys. Rev. C* **95**, 024303 (2017).
 - [17] B. A. Brown and W. A. Richter, *Phys. Rev. C* **74**, 034315 (2006).
 - [18] S. D. Głazek and K. G. Wilson, *Phys. Rev. D* **48**, 5863 (1993).
 - [19] F. Wegner, *Ann. Phys. (N.Y.)* **506**, 77 (1994).
 - [20] S. K. Bogner, R. J. Furnstahl, and R. J. Perry, *Phys. Rev. C* **75**, 061001(R) (2007).
 - [21] E. D. Jurgenson, P. Navrátil, and R. J. Furnstahl, *Phys. Rev. Lett.* **103**, 082501 (2009).
 - [22] S. Bogner, R. Furnstahl, and A. Schwenk, *Prog. Part. Nucl. Phys.* **65**, 94 (2010).
 - [23] K. Tsukiyama, S. K. Bogner, and A. Schwenk, *Phys. Rev. Lett.* **106**, 222502 (2011).
 - [24] H. Hergert, S. Bogner, T. Morris, A. Schwenk, and K. Tsukiyama, *Phys. Rep.* **621**, 165 (2016).
 - [25] F. A. Evangelista, *J. Chem. Phys.* **141**, 054109 (2014).
 - [26] J.-Y. Guo, *Phys. Rev. C* **85**, 021302(R) (2012).
 - [27] S. D. Głazek and J. Młynik, *Phys. Rev. D* **67**, 045001 (2003).
 - [28] P. Ring and P. Schuck, *The Nuclear Many-Body Problem* (Springer Science & Business Media, New York, 2004).
 - [29] T. D. Morris, N. M. Parzuchowski, and S. K. Bogner, *Phys. Rev. C* **92**, 034331 (2015).
 - [30] J. B. French, *Phys. Lett.* **26B**, 75 (1967).
 - [31] J. B. French, *Nucl. Phys. A* **396**, 87 (1983).
 - [32] S. S. M. Wong, *Nuclear Statistical Spectroscopy* (Oxford University Press, Oxford, 1986), Vol. 7.
 - [33] T. Dytrych, K. D. Sviratcheva, J. P. Draayer, C. Bahri, and J. P. Vary, *J. Phys. G* **35**, 123101 (2008).