Group-theoretical approach to interaction renormalization for \textit{ab initio} solutions of the nuclear problem

Kristina D. Sviratcheva\textsuperscript{1}, Jerry P. Draayer\textsuperscript{1}, Tomáš Dytrych\textsuperscript{1}
\textsuperscript{1} Department of Physics and Astronomy, Louisiana State University, Baton Rouge, LA 70803, USA

Abstract. For many problems in nuclear, high-energy and solid-state physics a crucial step toward a solution involves a diagonalization or simplification of the Hamiltonian of a many-body quantum-mechanical system. Problems of interest include renormalization of the Hamiltonian to accommodate excluded basis spaces, decoupling of a model space region of special interest from irrelevant configurations, or near-diagonalization to invoke perturbative treatments. In such applications, the Similarity Renormalization Group (SRG) approach (or \textit{flow equations}) can provide solutions where more conventional methods fail. We show that when SRG employs a near symmetry of a system, utilizing the Casimir invariant operators, it evolves the Hamiltonian of the system toward a (block-)diagonal form that can be realized in terms of a finite number of integrity basis operators. In particular, for atomic nuclei, an SRG flow equation that utilizes the SU(3) symmetry, which often dominates the nuclear dynamics, is found to naturally evolve a nucleon-nucleon (NN) interaction toward a block-diagonal form. A remarkable consequence is that a renormalized SU(3)-preserving many-body Hamiltonian expressed in terms of only the SU(3) integrity basis realizes energy spectra identical to the ones of the original realistic NN interaction, which reflects the low-energy symmetries as well as symmetry-breaking patterns of quantum chromodynamics. Such a scheme is especially suitable for \textit{ab initio} SU(3) symmetry-adapted shell model calculations, which can further allow for perturbative treatments of the nuclear interaction. Moreover, the use of symmetries dramatically reduces the size of the problem, as the flow equation can be rewritten in terms of SU(3) reduced matrix elements of the NN interaction. This is crucial for maintaining the unitarity of the SRG transformations that generate many-body interactions.

1. Introduction

Analogous to the Jacobi numerical method for diagonalization in a stepwise fashion, the Similarity Renormalization Group (SRG) or \textit{flow equations} approach has been designed as a nonperturbative renormalization/diagonalization method by Glazek and Wilson \cite{1, 2} and independently by Wegner \cite{3}. Recent studies of interest include quantum nonequilibrium systems \cite{4}, the sine-Gordon strong-coupling model \cite{5}, the SU(2) Lipkin model \cite{6}, the Hubbard model together with a focus on the electron-phonon problem \cite{7, 8}, and effective field theory for, e.g., quantum electro- and chromo-dynamics \cite{9, 10}.

In nuclear physics, modern realistic internucleon interactions tied to quantum chromodynamics (QCD) considerations currently limit \textit{ab initio} nuclear structure calculations \cite{11, 12, 13, 14} to slow convergence with increasing model spaces, restricted many-body correlations, or small nucleon numbers. While innovative \textit{ab initio} approaches (e.g., \cite{15, 16, 17}) attempt to address...
these limitations, the use of techniques for renormalization (e.g., Lee-Suzuki [18, 19], SRG [20], and UCOM [21]) of two-nucleon \((NN\) or 2\(N\)), and perhaps 3\(N\) and 4\(N\), interactions prove essential.

In this study we show that using symmetries that dominate the many-body dynamics yields controllable SRG-generated higher-order coupling terms (many-body forces), which are essential to retaining the unitarity of the SRG transformations and key to the method’s applicability. A novel perspective, based on the spectral distribution theory [22], provides further insight into the SRG approach. Specifically, 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 with coordinates specified by the independent matrix elements of \(H\). The \(\sigma_H\) vector “length” (specifying the interaction “strength”) is related to the Hilbert-Schmidt norm, \(\sigma^2_H = \langle (H - \langle H \rangle)(H - \langle H \rangle) \rangle\) with \(\langle \ldots \rangle \equiv \frac{1}{N_d} \text{Tr}(\ldots)\), while the spatial orientation of two operators, \(H\) and \(H'\), is given by their correlation coefficient (specifying the similarity between the two interactions), \(\zeta_{H,H'} = \frac{\langle (H - \langle H \rangle)(H' - \langle H' \rangle) \rangle}{\sigma_H \sigma_{H'}} = \cos \theta\), with \(\theta\) being the angle between \(H\) and \(H'\). Hence, the positive square root of \(\sigma_H^2\) is a natural measure of the size of the \(H\) operator and realizes the width (or spread) of the \(H\) eigenvalue distribution, namely, the smaller the width (the weaker the interaction), the more compressed the energy spectrum of \(H\). In the framework of spectral distribution theory, we present first estimates for the strength of the SRG-induced many-body forces for a general case [23]. Furthermore, a realization of the SRG-evolved Hamiltonian in terms of a finite set of integrity basis (IB) operators with usually known analytical matrix elements and reduced dimensions that capitalize on the use of symmetry make many-body SRG calculations feasible. Such a scheme applied to realistic \(NN\) interactions is especially suitable for \textit{ab initio} symmetry-adapted shell models as the interaction becomes prediagonalized in the basis while allowing for further perturbative treatments.

2. Theoretical Framework

The SRG concept performs a continuous sequence of \(U(s)\) infinitesimal unitary transformations of a \(H\) Hamiltonian that is generated by the antihermitian \(\eta\) operator, \(\eta^\dagger = -\eta\),

\[
H_s = U(s)HU(s)\dagger \text{ with } U(s) = e^{\eta s}, \tag{2.1}
\]

which preserves the trace and strength of the Hamiltonian, \(\langle H_s \rangle = \langle H \rangle\) and \(\sigma_{H_s} = \sigma_H\). The differential SRG procedure is based on the following class of equations,

\[
\frac{d}{ds} H_s = [\eta, H_s]. \tag{2.2}
\]

As shown below, the generator \(\eta\) is chosen in a way to drive the Hamiltonian toward a specific – usually, (block-)diagonal – form. In the framework of spectral distribution theory, for any general hermitian operator, \(C_s\), which varies with \(s\), Eq. (2.2) yields,

\[
\frac{d}{ds} \langle (C_s - \langle C_s \rangle)(H_s - \langle H_s \rangle) \rangle = \left\langle \frac{d(C_s - \langle C_s \rangle)}{ds} H_s \right\rangle + \left\langle C_s[\eta, H_s] \right\rangle
\]

\[
\sigma_H (\dot{\zeta}_{C_s,\zeta_{H_s,C_s}} + \sigma_{C_s} \zeta_{H_s,C_s}) = \left\langle \frac{d(C_s - \langle C_s \rangle)}{ds} H_s \right\rangle + \left\langle [H_s, C_s][\eta] \right\rangle, \tag{2.3}
\]

where we use that the trace of a commutator is zero \((\text{Tr}([\eta, H_s]) = 0)\). We consider two choices for \(C_s\), (i) \(C_s\) does not vary with \(s\) (fixed), and (ii) \(C_s\) is the diagonal part of \(H_s\), \(D_s\), as originally proposed by Wegner [3].
(i) \( C_s = C \) does not vary with \( s \) (fixed). Eq. (2.3) becomes,
\[
\sigma_H \sigma_C \dot{\zeta}_{H_s,C} = \left\langle [C, H_s] | H_s \right\rangle \eta.
\tag{2.4}
\]

(ii) \( C_s = D_s \) is the diagonal part of \( H_s \). As \( H_s = D_s + O_s \), where \( O_s \) is the traceless nondiagonal part of \( H_s \), the relations \( \langle D_s O_s \rangle = 0 \) and \( \sigma_H^2 = \sigma_D^2 + \sigma_O^2 \) hold. In this case, Eq (2.3) becomes,
\[
\sigma_H \sigma_D \dot{\zeta}_{H_s,D_s} = -\sigma_D \sigma_D + \left\langle \frac{d(D_s - \langle D_s \rangle)}{ds} H_s \right\rangle + \left\langle [D_s, H_s] \right\rangle \eta
\]
\[
= \left\langle D_s O_s \right\rangle + \left\langle [H_s, D_s] \right\rangle \eta
\]
\[
\sigma_H \sigma_D \dot{\zeta}_{H_s,D_s} = \left\langle [D_s, H_s] \right\rangle | \eta \rangle,
\tag{2.5}
\]

where we use that \( \sigma_{D_s} = \sigma_H \zeta_{H_s,D_s}, \sigma_{D_s} \sigma_{D_s} = \left\langle \frac{d(D_s - \langle D_s \rangle)}{ds} (D_s - \langle D_s \rangle) \right\rangle = \left\langle \frac{d(D_s - \langle D_s \rangle)}{ds} D_s \right\rangle \)
and \( \left\langle \frac{d(D_s - \langle D_s \rangle)}{ds} O_s \right\rangle = \langle D_s O_s \rangle = 0 \), as \( \sum_{ij} H_{s,ij} \delta_{ij} O_{s,ji} = 0 \) \( (O_{s,ii} = 0) \).

Clearly, for both cases, \( C_s = C \) (2.4) and \( C_s = D_s \) (2.5), by choosing,
\[ \eta = [C_s, H_s] \]
the rate of change of \( \zeta_{H_s,C_s} \) is always nonnegative \( (\langle \eta | \eta \rangle \geq 0) \),
\[ \frac{d}{ds} \zeta_{H_s,C_s} = \frac{\sigma_{\eta_s}^2}{\sigma_H \sigma_C} \geq 0, \]
\tag{2.7}

where the \( \eta_s \) strength is, \( \sigma_{\eta_s} = \sqrt{\left\langle [H_s, C_s] [C_s, H_s] \right\rangle} = \sqrt{2 \langle C_s^2 H_s^2 \rangle - 2 \langle C_s H_s C_s H_s \rangle} \). This dependence (2.7) is significant as it reveals that the \( \zeta_{H_s,C_s} \) correlation between \( H_s \) and \( C_s \) that is bounded from above monotonically increases until \( \sigma_{\eta_s}^2 \) is zero, that is until \( H_s \) commutes with \( C_s \) \( ([C_s, H_s] = 0) \) when \( \zeta_{H_s,C_s} \) is maximum. Hence, the \( \zeta_{H_s,C_s} \) evolution (2.7) with decreasing “decoupling” energy parameter \( \lambda_d = 1/\sqrt{s} \) manifests the increasing similarity between the evolved \( H_s \) and the \( C_s \), and equally, traces the dynamics of the decoupling between states of low-\( C_s \) eigenvalues from those with high-\( C_s \) eigenvalues. Therefore, if \( C_s \) is chosen to be diagonal in the representation of the initial \( H_s, H_s \) is driven toward a (block-)diagonal form in this representation. In the case of \( C_s = D_s, H_s \) is driven toward its diagonal part and eventually coincides with \( D_s \) when \( \zeta_{H_s,D_s} = 1 \). We choose \( C \) to be the second-order Casimir invariant, \( C_{s,3}^{su3} \), diagonal in a SU(3) shell model basis. Other choices for \( C \) include the diagonal part of \( H_s, D_s \) [3], as well as, for nuclear structure physics, the \( T_{rel} \) relative kinetic energy [20] and the free \( H_{HO} \) harmonic oscillator (HO) Hamiltonian.

Furthermore, in the case when \( C \) is a linear combination of the Casimir invariants of the symmetry under consideration [e.g., of the \( C_{s,3}^{su3} \) and the third-order \( C_{s,3}^{su3} \) for the rank two SU(3) group], the symmetry-based SRG approach offers an improvement over the use of the diagonal \( D_s \). Specifically, for \( \sigma_{\eta_s} \approx 0, H_s \) becomes a superposition of operators that respect the symmetry and therefore commutes with \( C \). These operators lie in a “plane” (symmetry plane) spanned by a countable number of integrity basis operators [24]. This remarkable result points to the fact that \( H_s \) can then be expressed as a finite polynomial in the generators and scalars of the symmetry. For nuclear dynamics, this implies that a many-body \( H_s \), that realizes an equivalent energy spectrum of a realistic \( NN \) interaction, \( H \) (or \( H_0 = H_{NN} \), can be chosen to be SU(3)-symmetric and expressed in terms of SU(3) generators and scalars, while reflecting the low-energy symmetry patterns of QCD inherent to the \( NN \) realistic interaction.
In short, the spectral distribution theory brings forward a geometrical interpretation of the SRG approach. Clearly, $\eta$ generates infinitesimal rotations of $H_s$ in a perpendicular multi-dimensional “plane”, which contains $H_s$ and $C$ together with any many-body operator $X$ that commutes with $C$ or $H_s$. This follows from the fact that $\zeta_{C_s,\eta} = 0$, $\zeta_{H_s,\eta} = 0$, and $\zeta_{X,\eta} = 0$, since $\text{Tr}(H_s\eta) = \text{Tr}(C[H_s,H_s]) = 0$ and $\text{Tr}(X\eta) = \text{Tr}([X,C]H_s) = 0$.

The discussions that follow refer to a fixed $C$ not varying with $s$ (such as $C_2^{\text{a}3}$, $C_3^{\text{a}3}$, $T_{\text{rel}}$, and $H_{\text{HO}}$) and may not apply to the diagonal $D_s$.

**Dimensionless SRG evolution** – In the framework of spectral distribution theory, a dimensionless SRG evolution is readily available. In particular, we introduce dimensionless unit operators, $H'_s = \frac{H_s}{\sigma_H}$ and $C' = \frac{C}{\sigma_C}$ ($\sigma_{H'_1} = 1$ and $\sigma_{C'} = 1$), and hence Eq. (2.2) becomes,

$$\frac{d}{ds} H'_s = \left[\left[ C', H'_s \right], H'_s \right],$$

(2.8)

with dimensionless $\eta'_s = [C', H'_s]$ and $s' = s\sigma_CC_H$, together with $\lambda_d = \frac{1}{\sqrt{s}} = \sqrt{\frac{\text{rel} \sigma_H}{s}}$ in units of energy. The correlation coefficient rate of change (2.7) is thus given by,

$$\frac{d}{ds} \zeta_{H'_s, C'} = \sigma_{s'}.\eta'_s^2.$$  

(2.9)

**Traceless operators** – Without loss of generality (w.l.o.g.), we can assume traceless $H_s$ and $C$ matrices, that is $\langle H_s \rangle = 0$ and $\langle C \rangle = 0$. This is because the SRG flow (2.2) is independent of these traces as a result of the unitarity of transformations ($\langle H_s \rangle = \langle H \rangle$ and hence, $d \langle H_s \rangle / ds = 0$) together with the fact that traces commute.

In what follows, we will use – w.l.o.g. as shown above – a dimensionless flow and traceless operators.

**3. Hierarchy of higher-order flow-generated terms**

For an infinitesimal transformation, dependent upon a small parameter $\epsilon$, of an operator $K$ that is generated by a hermitian operator $G$ and evolving continuously from the identity, $U = 1 - i\epsilon G$, the transformed $K' = UKU^\dagger = K - i\epsilon [G,K]$. Clearly, with $\eta = -i\epsilon$, one obtains the SRG rotations (2.1).

For finite unitary transformations (as used in the numerical flow evolutions), the interaction is rotated at a finite $\delta s = h$ dimensionless step,

$$H_{n+1} = e^{\hbar\eta_s} H_n e^{-\hbar\eta_s} = \sum_{k=0}^{\infty} \frac{\hbar^k}{k!} H_{n(k)}$$  

(3.1)

with $H_{n(k)} = [\eta_1, [\eta_2, \ldots, [\eta_k, H_n] \ldots]]$ or equivalently, $H_{n(k)} = [\eta_n, H_{n(k-1)}]$ with $H_{n(0)} = H_n$.

Here, the $k$-th term involves $k$ commutators yielding a many-body interaction of a strength $\sigma_{H_{n(k)}}$, which can be shown to be at the most of order of $(S_\eta)^{2k}$ for a $S_\eta$ upper bound of $\sigma_\eta$ (Appendix A).

Clearly, with a 1-body $C$ and a 2-body $H_0$ initial Hamiltonian, the first rotation renders $H_{0(1)}$ 3-body, $H_{0(2)}$ 4-body and etc. $H_{0(1)}$ is of particle rank 3, which includes 2-body interactions that are present in a flow evolved in a two-particle system ($A = 2$). However, such a flow does not take into account the pure 2-body part of the 3-body terms in $H_{0(1)}$. The lowest particle

1 A definite $\nu$ particle rank interaction (pure $\nu$-body interaction), e.g., for a scalar distribution, is a $U(N)$ irreducible tensor $H^\nu(\nu)$ of rank $\nu = 0, 1, \ldots, k$, such that for a $k$-body interaction, $H^k = \oplus H^\nu(\nu)$ and $N$ is the single-particle basis space dimension.
ranks (LPR) of the induced interaction that are not present in $H_0$ enter in $hH_0(1)$, while higher particle ranks, such as the next-to-LPR (NLPR) in $h^2H_0(2)$ and N$^2$LPR in $h^3H_0(3)$, are brought forward in the next terms. In general, for a $p_1$-b $C$ and a $p_2$-b $H_0$, the maximum particle rank of $H_n$ at $\mathcal{O}(h^k)$ is $K'(p_1 + p_2 - 2) + (2 - p_1)$.

It is sufficient to choose $hS^2_\eta < 1$ to observe a hierarchy of the many-body terms within a rotation and to evolve (2.2),

$$H_{n+1(I)} = H_{n+1} - H_n = hH_{n(1)} + \frac{h^2}{2!}H_{n(2)} + \frac{h^3}{3!}H_{n(3)} + \mathcal{O}(h^4).$$

(3.2)

As $H_{n(k+1)} = [\eta_n, H_{n(k)}]$, every two $H_{n(k+1)}$ and $H_{n(k)}$ are orthogonal (that is, $\langle H_{n(k+1)}H_{n(k)} \rangle = 0$) and in addition, $\langle H_{n(k+2)}H_{n(k)} \rangle = -\sigma^2_{H_{n(k+1)}}$. While $H_{n(2)}$ does not project onto $H_{n(1)}$, $H_{n(3)}$ contains $H_{n(1)}$-like contributions, $H_{n(3)} = w_nH_{n(1)} + \tilde{H}_{n(3)}$ with $w_n = \frac{\langle H_{n(3)}H_{n(1)} \rangle}{\sigma^2_{H_{n(1)}}} = -\sigma^2_{H_{n(2)}}$, where $\tilde{H}_{n(3)}$ is the $H_{n(3)}$ portion orthogonal to $H_{n(1)}$ (clearly, it is also orthogonal to $H_{n(2)}$). Hence,

$$H_{n+1(I)} = (1 + \frac{h^2}{3!}w_n)hH_{n(1)} + \frac{h^2}{2!}H_{n(2)} + \frac{h^3}{3!}H_{n(3)} + \mathcal{O}(h^4),$$

(3.3)

and the induced interaction strength at the $(n + 1)^{st}$ rotation is given by $\sigma^2_{H_{n+1(I)}} = \langle H_{n+1(I)}^2 \rangle$,

$$\sigma^2_{H_{n+1(I)}} = (1 + \frac{h^2}{3!}w_n)^2h^2\sigma^2_{H_{n(1)}} + \frac{h^4}{4}\sigma^2_{H_{n(2)}} + \mathcal{O}(h^6),$$

$$= (1 + \frac{h^2}{3}w_n)h^2\sigma^2_{H_{n(1)}} + \frac{h^4}{4}\sigma^2_{H_{n(2)}} + \mathcal{O}(h^6).$$

(3.4)

The first term in (3.4) is of the $H_{n(1)}$ particle rank, while the second term introduces higher-order couplings. The strengths of the interactions in (3.3) are related as, $\sigma^2_{H_{n+1(I)}} = h^2\sigma^2_{H_{n(1)}} - \frac{h^4}{12}\sigma^2_{H_{n(2)}} + \mathcal{O}(h^6)$.

To estimate the LPR contribution to $hH_{n(1)}$, the latter can be expressed as [using (3.1)],

$$hH_{n(1)} = hH_{n-1(1)} + h^2V_{n-1(2)} + h^3V_{n-1(3)} + \mathcal{O}(h^4),$$

$$V_{n-1(2)} = H_{n-1(2)} + [C, H_{n-1(1)}],$$

$$V_{n-1(3)} = \frac{1}{2}H_{n-1(3)} + [C, H_{n-1(1)}],$$

and thus directly related, in first order, to the LPR in $hH_{0(1)}$. Similarly to the orthogonalization we perform above, one can identify the $H_{n(1)}$-like contributions of $V_{n(2)}$ and $V_{n(3)}$,

$$V_{n(2)} = q_nH_{n(1)} + \tilde{V}_{n(2)}; \quad q_n = \frac{\langle H_{n(1)}V_{n(2)} \rangle}{\sigma^2_{H_{n(1)}}},$$

$$V_{n(3)} = r_nH_{n(1)} + \tilde{V}_{n(3)}; \quad r_n = \frac{\langle H_{n(1)}V_{n(3)} \rangle}{\sigma^2_{H_{n(1)}}},$$

(3.6)

where $\tilde{V}_{n(2)} [\tilde{V}_{n(3)}]$ is the $V_{n(2)} [V_{n(3)}]$ portion orthogonal to $H_{n(1)}$, and thus obtain,

$$hH_{n(1)} = p_nhH_{n-1(1)} + h^2\tilde{V}_{n-1(2)} + h^3\tilde{V}_{n-1(3)} + \mathcal{O}(h^4),$$

$$p_n = 1 + hq_{n-1} + h^2r_{n-1}.$$
Note that \( p_n \) gives the projection of \( H_{n(1)} \) onto \( H_{n-1(1)} \), \( p_n = \langle H_{n-1(1)} H_{n(1)} \rangle / \sigma_{H_{n-1(1)}}^2 \). It follows that,

\[
\begin{align*}
\hbar^2 \sigma_{H_{n(1)}}^2 &= p_n^2 \hbar^2 \sigma_{H_{n-1(1)}}^2 + h^4 \sigma_{\tilde{V}_{n-2(2)}}^2 + O(h^5) \\
&= ((1 + h q_n - 1)^2 + 2h^2 r_n - 1) \hbar^2 \sigma_{H_{n-1(1)}}^2 + h^4 \sigma_{\tilde{V}_{n-2(2)}}^2 + O(h^5),
\end{align*}
\]

where, to \( O(h^3) \), \( p_n^2 = (1 + h q_n - 1)^2 + 2h^2 r_n - 1 \) with

\[
q_n = \frac{d}{ds} \ln(\sigma_{H_{n(1)}}) \bigg|_n \quad \text{and} \quad r_n \approx -\frac{\sigma_{H_{n(2)}}^2}{\sigma_{H_{n(1)}}^2}. \quad (3.9)
\]

This follows from, \( q_n \sigma_{H_{n(1)}}^2 = \langle H_{n(1)} V_{n(2)} \rangle = \langle H_{n(1)} | \{ C, H_{n(1)} \} | H_{n} \rangle = \langle H_{n(1)} | \frac{d}{ds} \left[ H_{n(1)} \right] \rangle_{H_{n}} \bigg|_n \approx \frac{1}{2} \frac{d}{ds} \sigma_{H_{n(1)}} \bigg|_n \), where we use that \( \frac{d}{ds} \left[ H_{n(1)} \right] = H_{n(1)}, \frac{d}{ds} \left[ H_{n(1)} \eta_n, H_{n} \right] = 0 \), together with an approximate \( r_n \) value, for which typically \( \langle H_{n(1)} V_{n(3)} \rangle \approx \langle H_{n(1)} H_{n(3)} \rangle \). Note that as \( h \to 0 \) (infinitesimal rotations), the \( h^4 \) terms in (3.8) vanish and the approximation in \( r_n \) becomes irrelevant.

Therefore, the main contribution to \( H_{n(1)} \) is due to the LPR interactions that emerge in \( H_{0(1)} \),

\[
\begin{align*}
\hbar^2 \sigma_{H_{n(1)}}^2 &= \hbar^2 \sigma_{H_{0(1)}}^2 \prod_{k=1}^{n} p_k^2 + h^4 \left( \sum_{k=2}^{n} \sigma_{\tilde{V}_{k-2(2)}}^2 \prod_{l=k}^{n} p_l^2 + \sigma_{\tilde{V}_{n-1(2)}}^2 \right) + O(n h^5), \\
&= \hbar^2 \sigma_{H_{0(1)}}^2 \prod_{k=1}^{n} p_k^2 + n h^4 \sigma_{\tilde{V}_{0(2)}}^2 + O(n h^5), \quad (3.10)
\end{align*}
\]

where we use that, \( p_k^2 = 1 + O(h) \) in the \( h^4 \)-term, together with the fact that, to \( O(h^6) \), \( h^4 \sigma_{\tilde{V}_{n(2)}}^2 \sim h^4 \sigma_{\tilde{V}_{n-1(2)}}^2 \) and hence, related to the NLPR of \( \tilde{V}_{0(2)} \). The induced interaction strength (3.4) at the \((n+1)\)st rotation is then,

\[
\sigma_{H_{n+1(1)}}^2 = \hbar^2 \sigma_{H_{0(1)}}^2 \left( 1 + \frac{\hbar^2}{3} w_n \right) \prod_{k=1}^{n} p_k^2 \\
\begin{aligned}
\equiv & \sigma_{n, \text{LPR}}^2 \\
+ & nh^4 \sigma_{\tilde{V}_{0(2)}}^2 + \frac{h^4}{4} \sigma_{H_{0(2)}}^2 + O(n h^5),
\end{aligned} \quad (3.11)
\]

with a major contribution (\( \sim h^2 \)) of the LPR induced interactions (\( \sigma_{n, \text{LPR}}^2 \)) and a much smaller contribution (\( \sim h^4 \)) of the NLPR induced interactions (\( \sigma_{n, \text{NLPR}}^2 \)).

To estimate the total strength of the \((N)\)LPR interaction, \( \sigma_{(N)\text{LPR}} \), induced during the SRG flow evolved to \( \lambda_{d, \text{min}} \) (in units of energy), the induced interactions at each rotation are summed as aligned ‘vectors’ (that lie on \( H_{0(1)} \) regardless of the sign of their projection), which is an upper bound, \( |a + b| \leq |a| + |b| \), while the sum of the perpendicular vectors, projections on \( H_{0(1)} \) and projections on \( \tilde{V}_{0(2)} \), give the total induced interaction strength, \( \sigma_I \),

\[
\begin{align*}
\sigma_{(N)\text{LPR}} &= \sum_{n=0}^{n_{\text{max}}-1} \sigma_{n,(N)\text{LPR}} \\
\sigma_I &= \sqrt{\sigma_{\text{LPR}}^2 + \sigma_{\text{NLPR}}^2}. \quad (3.12)
\end{align*}
\]
where $n_{\text{max}} h = \sigma_H \sigma_C / \lambda^2_{d,\text{min}}$ for dimensionless $h$ and the error term for $\sigma_{(N)\text{LPR}}$ is of order of $n_{\text{max}}^2 h^3 \sim O(h)$. Note that $\sigma_{\text{LPR}}$ is of order of $n_{\text{max}} h$, which is a constant for given $\lambda^2_{d,\text{min}}$. For infinitesimal rotations, $h \to 0$ and $n_{\text{max}} h = \sigma_H \sigma_C / \lambda^2_{d,\text{min}}$, $\sigma_{\text{NLPR}} \to 0$. The only contribution to $\sigma_I$ is due to the LPR interactions. The latter include the LPR component of the NLPR $V_0(t)$ (that enters through $q_n$), while contributions from NNLR ($(n_n$ and $w_n$) vanish.

4. Flow dynamics and estimates for the strengths of the LPR and NLPR induced higher-order coupling terms

To obtain estimates for the total strength of the (N)LPR induced interaction, one needs to determine $p_n$ ($q_n$ and $r_n \approx w_n$ (3.9)), that is, $\sigma_{H(1)}$, $\sigma_{H(2)}$, and the rate of change of $\sigma_{H(1)}$. We employ $\sigma_{H(k)}$ typically $\sim \sigma_{n_k}$ (analogous to their $S_{n_k}^2$ upper limits) and an approximate upper limit of $\sigma_{n_k}$,

$$\sigma_{n_k} \approx \frac{2\sigma_{n_0}}{1 + \zeta_{H_0,C}} e^{-\frac{\sigma_{n_0}^2 H_0 \sigma_C}{1 - \zeta_{H_0,C}}},$$

(4.1)

which can be deduced from (2.7) and the smallest decrease rate of $\sigma_{n_k}$ (Appendix B),

$$\frac{d}{ds} \sigma_{n_k}^2 \leq -\frac{2\sigma_{n_k}^4}{\sigma_H \sigma_C} \frac{\zeta_{H,C}}{1 - \zeta_{H,C}}.$$

(4.2)

where w.l.o.g. we assume $\zeta_{H_0,C} \geq 0$. This approximation excludes local increases in $\sigma_{n_k}$, and uses that typically for near symmetries (strongly correlated C and the evolved $H_k$), $\zeta_{H_k,C} \approx \zeta_{H_k,C,0} \zeta_{H_k,C}$. In particular, for $\delta = 0.01$, $\bar{\sigma}_{H(0)} \approx \bar{\sigma}_{H(0)} \approx 1$ (with $h \equiv \delta / \sigma_{n_0}^2$ and $\bar{\sigma}_{H(0,k)} \equiv \sigma_{H(0,k)} / \sigma_{n_0}$) and a typical $\zeta_{H_0,C} \approx 0.2$, the total NLPR induced during an infinitely evolved flow turn out to be only 0.45% of the total induced interactions ($\sigma_{\text{LPR}}^2 / \sigma_{\text{LPR}}$). This percentage is proportional to $\delta$ and $\bar{\sigma}_{H(0,2)}$, and hence for larger $\bar{\sigma}_{H(0,2)}$ smaller $\delta$ steps are preferable. It is also possible to estimate the contribution of 3-b interactions to the induced $\sigma_{\text{LPR}}$. Namely, three-shell $T = 1$ calculations ($s$, $p$ and $sd$) with random 1-b $C$ and 2-b $H_0$ initial interaction with $\zeta_{H_0,C} = 0.2$ reveal that $\sigma_{H(0,2)}^2$ contains around 40% (60%) 3-b (2-b) interactions (incidentally, the pure 2-b part of the 3-b interaction is only $\approx 3\%$). This implies that for the example parameters (and with dimensionless $\sigma_{H(C)} = 1$), the induced 2-b LPR interaction strength is $\sigma_{\text{LPR} - 2b} \approx 0.62 (59.73\%$ of the total induced $\sigma_{H(1)}^2$), the induced 3-b LPR interaction strength is $\sigma_{\text{LPR} - 3b} \approx 0.51 (39.82\%$ of $\sigma_{H(1)}^2$), and $\sigma_{\text{NLPR}} = 0.05$, which includes 4-body interactions. These strengths further decrease for larger $\zeta_{H_0,C}$. Therefore, while it is clear that SRG evolving $H_N$ with a 1-b $C$ in a $A = 2$ system neglects 3-b terms with a contribution $\lesssim 67\%$ as compared to the SRG-induced 2-b interactions and hence not suitable for $A \geq 3$ applications, SRG evolved in a $A = 3$ system will neglect, in addition to an even smaller contribution of higher particle rank interactions, net 4-b forces of significance of less than a percent $(\sigma_{\text{NLPR}})$ together with the pure 3-b part of the 4-b NLPR forces (note that the dominant 3-b NLPR forces are accounted for). The forces neglected appear to be insignificant in applications of such renormalized interactions to $A = 4$ [25], further rendering applications to $A > 4$ systems feasible. Note that the second in importance term $(\hbar H_{0(1)})$ is 5-b if evolving $H_{NN+3N}$ requiring at least $A = 5$ SRG calculations. This term is 4-b for evolving $H_N$ with the 2-b $C_{2}^{su3}$. Fortunately, in the SU(3) case, the use of symmetry renders 4-body terms manageable.
Figure 1. SRG evolution ($J = T = 0$, 8 shells) for $\lambda_d = \infty$, 31.6, 10, 3.2 and 1 MeV of $T_{rel} +$ (a) AV18 and (b) N$^3$LO $NN$ bare interactions. Nonzero matrix elements (filled squares) are shown for SU(3)-coupled two-nucleon basis states, ordered by increasing $C_{s^2u^3}$ eigenvalues.

The $C_{s^2u^3}$-SRG is applied to a general 2-b interaction in a representation of a SU(3)-coupled HO basis (using conventional labels and $\Gamma = JT$), $|n_r n_u \omega \kappa (LS) \Gamma M_T\rangle = \frac{\{a^\dagger_{n_r} \times a^\dagger_{n_u}\}^{\omega (LS) \Gamma M_T\}}{\sqrt{1 + \delta_{nr, nu}}}$ with SU(3) quantum numbers, $\omega \equiv (\lambda \mu) = (n_r 0) \times (n_u 0)$, and $\kappa$ multiplicity of $L$ for a given $\omega$. This basis is obtained via a unitary transformation from the $JT$-coupled HO basis, $|ru \Gamma M \rangle$ with $r(u) = \{n(l \frac{1}{2}) j \frac{1}{2}\}$, and yields the (isoscalar) Hamiltonian matrix elements ($\chi = n_r n_u$ for a two-particle system), $V^\kappa_{fi} = \langle \chi_f \omega_f \kappa_f (L_f S_f) \Gamma \parallel H \parallel \chi_i \omega_i \kappa_i (L_i S_i) \Gamma \rangle / \sqrt{2\Gamma + 1}$. The $C_{s^2u^3}$ ($C_{s^3u^3}$ and $H_{\text{HO}}$) is diagonal in this basis and can be used to drive $H$ toward a block-diagonal form.

The two-particle $C_{s^2u^3}$-SRG method, performed separately for each $\Gamma$, is applied to various realistic $NN$ interactions, such as CD-Bonn ($\hbar \Omega=15$ MeV) and N$^3$LO (11 MeV) [26, 27], as well as JISP16 (15 MeV) [28] and AV18 (18 MeV) [29], with the relative kinetic energy added prior to the SRG transformation. As an illustrative example, we consider $6\hbar \Omega$ for 'p-shell' nuclei (Fig. 1). Using the aforementioned estimates based only on $C_{s^2u^3}$ and $H_{\text{NN}}$ initial properties, it is expected that, e.g., for N$^3$LO evolved to $\lambda_d = 1$ MeV with $\delta \sim 0.001$, the net NLPR contribution to the total induced interaction is less than 0.8%. In Fig. 1, the order of states is chosen in increasing $C_{s^2u^3}$ eigenvalues, that is, in increasing deformation. Typically, large deformations involve high-energy configurations, which correspond to large excitation numbers $N$. Hence, the SRG brings forward decoupling of higher-energy configurations (large $N\hbar \Omega$) from the low-energy ones.

5. Conclusions
We introduced symmetry considerations into the Similarity Renormalization Group (SRG) theory for nuclear physics applications. Specifically, invariants of SU(3), which is a symmetry that is known to dominate the dynamics, were used to evolve the SRG flow. First we gave quantitative estimates for the strength of the SRG-induced many-body interactions for a general flow, and then showed that an application of the SU(3)-SRG approach to various two-nucleon interactions decouples low-energy configurations that are especially relevant for the regime of ordinary bound systems from higher-energy ones, with manageable induced many-body forces.

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**Appendix A. Estimate for the strength of the SRG generator and \( H_{s(1)} \)**

To estimate the upper limit of the \( \eta_s = [C, H_s] \) strength,

\[
\sigma_{\eta_s}^2 = - \langle \eta_s \eta_s \rangle = 2 \langle C^2 H_s^2 \rangle - 2 \langle CH_s CH_s \rangle \tag{A.1}
\]

we use bounds of correlation coefficients,

\[
-1 \leq \zeta_{H_s C, CH_s} = \frac{\langle CH_s CH_s \rangle - \langle CH_s \rangle^2}{\sigma_{CH_s}^2} \leq 1,
\]

\[
-1 \leq \zeta_{C^2, H_s^2} = \frac{\langle C^2 H_s^2 \rangle - \langle C^2 \rangle \langle H_s^2 \rangle}{\sigma_{C^2} \sigma_{H_s^2}} \leq 1 \tag{A.2}
\]

and

\[
\sigma_{C^2}^2 \leq \langle C^2 H_s^2 \rangle - \langle CH_s \rangle^2. \tag{A.3}
\]

Hence, \( \sigma_{\eta_s}^2 \leq 4 \langle C^2 H_s^2 \rangle \leq 4 (\sigma_{C^2} \sigma_{H_s^2} + \langle C^2 \rangle \langle H_s^2 \rangle) \). During a flow with a \( s \)-independent \( C \), the strength of \( \eta_s \) for traceless \( C \) and \( H_s \) is found to have a \( S_\eta \) upper bound,

\[
\sigma_{\eta_s} \leq S_\eta = 2 \sigma_{C^2} \sigma_{H_s} \sqrt{\left( \mathcal{M}^{(4)} - 1 \right) \left( \mathcal{M}^{(4)} - 1 \right) + 1}, \tag{A.4}
\]

where the \( k \)-th spectral moment of an operator \( K \) (or \( H_s \)) scaled by \( \sigma_K \) is \( \mathcal{M}_K^{(k)} = \frac{1}{\sigma_K^k} \langle (K - \langle K \rangle)^k \rangle \). If an operator follows a Gaussian distribution, \( \mathcal{M}^{(4)} = 3 \), \( \mathcal{M}^{(6)} = 15 \), and \( \mathcal{M}^{(8)} = 105 \). Clearly, the second moment is always \( \mathcal{M}^{(2)} = 1 \) and for the unitary transformation of \( H, \mathcal{M}_H^{(k)} = \mathcal{M}_H^{(k)} \) and \( \sigma_{H_s} = \sigma_H \). This is an important result, as spectral moments need to be calculated only for the initial \( H \).

The moments for \( C_2^{(8)} \) and \( H \) are estimated for the 8-shell \( JT \)-coupled scheme of various realistic interactions, such as CD-Bonn (\( \hbar \Omega = 15 \text{ MeV} \)), N\( ^3 \)LO (11 MeV) [26, 27] and JISP16 (15 MeV) [28], with the relative kinetic energy added. In addition, the \( C_2^{(8)} \) analytical form is used to calculate moments in \( JT \)-coupled scheme up through \( N_{\text{max}} = 100 \), which agrees with the 8-shell calculations for \( C_2^{(8)} \). Hence, estimates for \( H \) in larger spaces are expected to remain of the same order. The spectral moments calculated are typically less than,

\[
\mathcal{M}_C^{(4)} C_2^{(8)} \sim 3, \mathcal{M}_C^{(6)} C_2^{(8)} \sim 15, \mathcal{M}_C^{(8)} C_2^{(8)} \sim 10^2, \mathcal{M}_H^{(4)} \sim 10, \text{ and } \mathcal{M}_H^{(6)} \sim 10^2. \tag{A.5}
\]

These estimates are used to provide upper limits for various strengths.

For example, the maximum strength of the dimensionless \( \eta_s \) is found from (A.4) and (A.5) to be \( S_\eta \sim 5 \) for \( C = C_2^{(8)} \). Similarly, the \( \sigma_{H_{s(1)}} \) strength of \( H_{s(1)} = dH_s/ds \) is less than,

\[
\sigma_{H_{s(1)}} \lesssim S_{H_{s(1)}} = 4 \sigma_{C^2} \sigma_{H_s}^2 \left( \sqrt[4]{\mathcal{M}_C^{(8)} \mathcal{M}_H^{(4)} + \mathcal{M}_C^{(4)} \mathcal{M}_H^{(6)}} \right)^{1/4}, \tag{A.6}
\]

which gives the estimate for the upper bound \( S_{H_{s(1)}} \sim S_\eta^2 \) for \( C = C_2^{(8)} \) and the realistic \( NN \) interactions under consideration (A.5).
Appendix B. Rate of change of $\sigma_{\eta_s}$

The rate of change of $\sigma_{\eta_s}$ is given as,

$$\frac{1}{2} \frac{d}{ds} \sigma_{\eta_s}^2 = - \left( \langle \eta_s \frac{d \eta_s}{ds} \rangle = - \left( C \frac{dH_s}{ds}, \eta_s \right) = \langle H_{s(2)} C \rangle \right)$$

$$\approx \sigma_C \sigma_{H_{s(2)}} \zeta_{H_{s(2)}, H_s \zeta_{H_s, C}} = - \frac{\sigma_C \sigma_{H_{s(1)}}^2}{\sigma_H} \zeta_{H_{s(1)}, C},$$

(B.1)

where we use that $\zeta_{H_{s(2)}, C} \approx \zeta_{H_{s(2)}, H_s \zeta_{H_s, C}}$ and $\sigma_{H_{s(2)} \zeta_{H_{s(2)}, H_s}} = \frac{1}{\sigma_H} \langle H_s H_{s(2)} \rangle = - \frac{\sigma_{H_{s(1)}}^2}{\sigma_H}$.

The smallest decrease of $\eta_s$ is given by the lower bound of $\sigma_{H_{s(1)}}$, which can be derived from,

$$\sigma_{\eta_s}^2 = - \langle \eta_s [C, H_s] \rangle = \langle CH_{s(1)} \rangle \leq \sigma_C \sigma_{H_{s(1)}} \sqrt{1 - \zeta_{H_s, C}}.$$  \hspace{1cm} (B.2)

This follows from $\zeta_{C, H_{s(1)}} = \zeta_{C, H_{s(1)}}, \zeta_{H_{s(1)}, H_s(s(1))} \leq \sin \theta_s$, where $H_{s(1)}$ is the projection of $H_{s(1)}$ in the $(H_s, C)$ plane. The angle between $H_{s(1)}$ and $C$ is $\frac{\pi}{2} - \theta_s$ $(H_{s(1)})$ is perpendicular to $H_s$ and $\cos \theta_s = \zeta_{H_s, C})$. Hence, $-\sigma_{H_{s(1)}}^2 \leq - \frac{\sigma_{\eta_s}^4}{\sigma_C^2 (1 - \zeta_{H_s, C})}$ and,

$$- \frac{\sigma_C \sigma_{H_{s(1)}}^2}{\sigma_H} \zeta_{H_s, C} \leq - \frac{\sigma_{\eta_s}^4}{\sigma_H \sigma_C} \frac{1}{1 - \zeta_{H_s, C}},$$

(B.3)

which together with (B.1) yields (4.2).

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