Towards *Ab-Initio* Nuclear Structure Calculations Beyond the p-Shell ⋆

Robert Roth

Institut für Kernphysik, Technische Universität Darmstadt,
Schlossgartenstr. 9, 64289 Darmstadt, Germany

Abstract

Recent developments in modern nuclear structure theory regarding the construction of phase-shift equivalent effective interactions and their use in *ab initio* calculations are discussed. Two methods for the construction of tamed interactions via unitary transformations are reviewed and compared: the Unitary Correlation Operator Method and the Similarity Renormalization Group. Furthermore, we present a simple importance truncation scheme within the no-core shell model, which gives access to nuclei well beyond the p-shell. Using the interactions discussed before, we show results for ground-state energies of closed-shell nuclei up to ^{40}Ca.

Key words: nuclear structure theory, effective interactions, no-core shell model
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1. Introduction

One of the prime goals of modern nuclear theory is to gain insight into the multitude of nuclear structure phenomena throughout the nuclear chart using a consistent theoretical framework with a direct link to the fundamental theory of strong interactions. Though low-energy quantum chromodynamics (QCD) will not be solved directly for a nuclear many-body problem for the forseeable future, important steps towards a truly QCD-based nuclear structure theory are being made. From the point of view of conventional nuclear structure theory the low-energy dynamics of quarks and gluons determines the interaction between nucleons. There are recent attempts to directly extract a nucleon-nucleon interaction from lattice QCD calculations of the two-nucleon system [1]. A more established strategy for constructing a QCD-motivated nuclear interaction is

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provided by chiral effective field theory. Based on a chiral Lagrangian, which includes the long-range pion dynamics explicitly and absorbs short-range physics in contact terms, consistent two- and three-nucleon interaction have been derived [2,3].

The challenge now is to employ these interaction in nuclear structure calculations throughout the nuclear chart. Apart from the lightest nuclei, the available approaches for the treatment of the many-body problem are generally not able to provide converged results based on traditional realistic interactions like the Argonne V18 potential [4] or the recent chiral interactions. For this reason, 'effective' interactions which are derived from the 'bare' interactions using similarity transformations are an important intermediate step. Among those transformation methods are the Lee-Suzuki transformation used extensively in the context of the no-core shell model [5,6] and renormalization group methods leading to the $V_{\mathrm{low}k}$ low-momentum interaction [7]. We are going to discuss two alternative methods, the Unitary Correlation Operator Method and the Similarity Renormalization Group in the following section.

2. Unitarily Transformed Realistic Interactions

The description of short-range correlations poses a particular problem when solving the nuclear many-body problem based on conventional realistic interactions. As the wavefunction of the deuteron indicates, the short-range repulsion of the potential suppresses the two-body density at small interparticle distances and the tensor force generates the D-wave admixture. These features are also present in exact solution of the many-nucleon problem. In terms of an expansion of the exact eigenstates in a basis of Slater determinants, e.g. in the context of the no-core shell model in a finite $N_{\mathrm{max}}\hbar\Omega$ space, a huge number of basis states involving high-lying states are required for an adequate representation of these correlated states. Apart from the lightest nuclei this is computationally not feasible. For heavier nuclei we rely on simplified model spaces, which cannot account for short-range correlations and thus prohibit the direct used of 'bare' realistic interactions.

One strategy to tackle this problem is to 'tame' the initial interaction using a unitary transformation. The transformation has to suppress the components of the interaction which generate short-range correlations. In terms of many-body matrix elements of the Hamiltonian, this can be viewed as a pre-diagonalization leading to a substantial improvement of the convergence behavior in a no-core shell model picture. For this purpose, only the system- and state-independent short-range part of the interaction-induced correlations needs to be considered—residual long-range correlations can be described quite efficiently within simple model spaces.

These transformations can be constructed such that the experimentally constrained on-shell properties of the initial potential, i.e. the asymptotic phase shifts, are exactly preserved. The resulting tamed potential thus is phase-shift equivalent by construction and can be viewed as a realistic interaction in its own right.

2.1. *Unitary Correlation Operator Method*

The idea of the Unitary Correlation Operator Method (UCOM) [8,9] is to explicitly construct a unitary operator C, which imprints the dominant short-range correlations onto an uncorrelated many-body state $|\Psi\rangle$ via the transformation

$$|\widetilde{\Psi}\rangle = \mathrm{C}\,|\Psi\rangle\ . \tag{1}$$

Already the deuteron allows us to identified the two dominant types of short-range correlations that C has to account for: (i) central correlations induced by the short-range repulsion of the NN interaction which suppress the two-body density at short interparticle distances; (ii) tensor correlations induced by the strong tensor force which generates the D-wave admixture or, in other terms, a correlation between the relative spatial orientation of the two nucleons and their spins.

Guided by this physical picture of the origin and the structure of central and tensor correlations, we can construct unitary operators for describing them. The central correlations can be generated by a radial shift in the relative coordinate of a nucleon-pair. Pictorially speaking, if two nucleon are within the region of the short-range repulsion, then the transformation has to push then apart. This kind of distance-dependent shift is described by the unitary operator

$$\mathrm{C}_r = \exp\Big[-\mathrm{i} \sum_{i<j} \mathrm{g}_{r,ij} \Big] \qquad \text{with} \qquad \mathrm{g}_r = \frac{1}{2}[s(\mathrm{r})\mathrm{q}_r + \mathrm{q}_r s(\mathrm{r})] \;, \tag{2}$$

where $\mathrm{q}_r = \frac{1}{2}[\mathbf{q}\cdot(\mathbf{r}/\mathrm{r}) + (\mathbf{r}/\mathrm{r})\cdot\mathbf{q}]$ is the radial component of the relative momentum $\mathbf{q}$ of a particle pair. The function $s(r)$ determines the distance-dependence of the shift and is determined for each spin-isospin channel from a variational calculation in the two-body system.

The unitary operator inducing tensor correlations has to reflect the non-central nature of the tensor force in order to generate admixtures of state with relative orbital angular momentum $L \pm 2$. This is achieved with the following operator

$$\mathrm{C}_\Omega = \exp\Big[-\mathrm{i} \sum_{i<j} \mathrm{g}_{\Omega,ij} \Big] \qquad \text{with} \qquad \mathrm{g}_\Omega = \frac{3}{2}\vartheta(\mathrm{r})\big[(\boldsymbol{\sigma}_1\cdot\mathbf{q}_\Omega)(\boldsymbol{\sigma}_2\cdot\mathbf{r}) + (\mathbf{r}\leftrightarrow\mathbf{q}_\Omega)\big] \;, \tag{3}$$

where $\mathbf{q}_\Omega = \mathbf{q} - \frac{\mathbf{r}}{\mathrm{r}}\,\mathrm{q}_r$ is the component of the relative momentum $\mathbf{q}$ perpendicular to $\mathbf{r}$. Similar to the central correlator, $\vartheta(r)$ describes the magnitude of the transformation as a function of distance.

The combined effect of the two transformations $\mathrm{C} = \mathrm{C}_\Omega \mathrm{C}_r$ on a simplistic relative wavefunction in the deuteron channel is illustrated in Fig. 1. We start from a smooth $L = 0$ wavefunction, which represents an uncorrelated state of a limited model space. The unitary transformation with the central correlation operator C_r creates the correlation hole at short interparticle distance by shifting the probability amplitude to larger distances. The tensor correlation operator C_Ω creates the $L = 2$ admixture out of the initial $L = 0$ state with an radial shape determined by the function $\vartheta(r)$. In order to reconstruct the full deuteron wavefunction the tensor correlation function $\vartheta(r)$ has to be long-ranged (dashed curves). These long-range tensor correlations are an artifact of the two-body system—embedded into a many-body system the long-range tensor correlations will be destroyed by tensor interactions with other nucleons. We therefore constrain the range of the tensor correlation function (solid curve) and use the value of the volume integral $I_\vartheta = \int \mathrm{d}r r^2 \vartheta(r)$ as a parameter, which will be fixed in subsequent few-body calculations.

Using the explicit form of the correlation operator C, we can directly formulate the unitarily transformed Hamiltonian in two-body space (2B)

$$\widetilde{\mathrm{H}} = \mathrm{C}^\dagger\,\mathrm{H}\,\mathrm{C} = \mathrm{C}^\dagger(\mathrm{T}+\mathrm{V})\mathrm{C} \overset{\text{2B}}{=} \mathrm{T} + \mathrm{V}_{\text{UCOM}} \;, \tag{4}$$

which defines the tamed or correlated two-body interaction V_{UCOM}. We will come back to the induced three-body contributions lateron. The fact that C is given in an explicit operator representation is very convenient: It allows us to derive a closed operator form of the correlated interaction V_{UCOM}. Furthermore, operators of other observables, e.g. densities, form factors, transition amplitudes, and exchange currents, can be correlated consistently without additional effort.

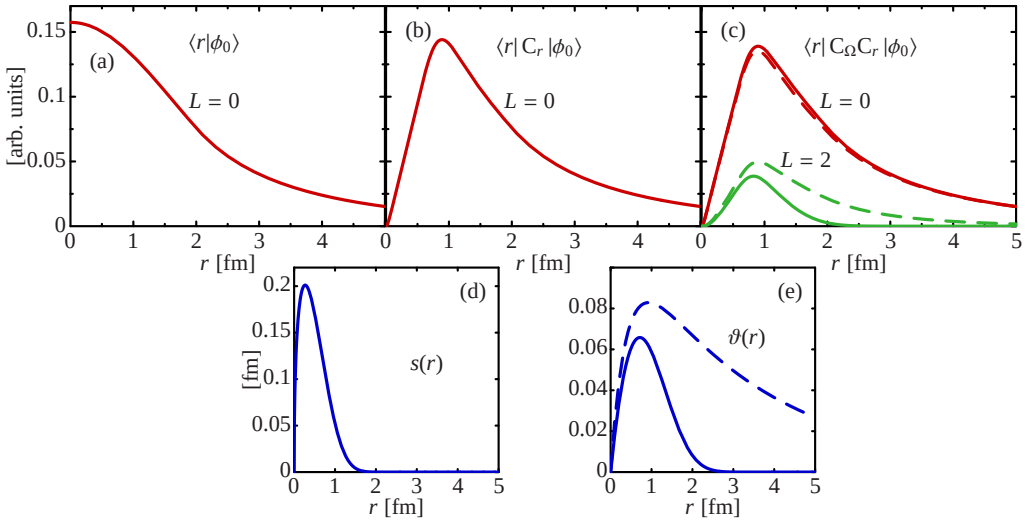

Fig. 1. Construction of the deuteron wavefunction in the UCOM framework. Starting from a smooth uncorrelated wavefunction (a) the subsequent application of the central (b) and tensor correlation operator (c) leads to a realistic deuteron wavefunction. The functions $s(r)$ and $\vartheta(r)$ determining the distance dependence of the transformations are shown in panels (d) and (e), respectively.

As mentioned earlier, the tamed interaction $\mathrm{V_{UCOM}}$ is phase-shift equivalent to the original potential but has a different off-shell behavior. In an operator representation, higher-order momentum operators and momentum-dependent tensor operators appear, which are not present in the usual parameterizations of realistic potentials.

2.2. *Similarity Renormalization Group*

The Similarity Renormalization Group (SRG) as a second method using unitary transformations to tame the interaction starts from a completely different background. Originally proposed by Wegner [10,11] in the context of solid-state systems, it aims at the pre-diagonalization of the Hamiltonian with respect to a given basis using renormalization group flow equations. Denoting the flow parameter α, the evolution of the Hamiltonian is described by the flow equation [12]

$$\frac{d\bar{\mathrm{H}}(\alpha)}{d\alpha} = [\eta(\alpha), \bar{\mathrm{H}}(\alpha)]\,, \qquad \bar{\mathrm{H}}(0) = \mathrm{H}\,. \tag{5}$$

Formally we can express the evolved Hamiltonian $\bar{\mathrm{H}}(\alpha)$ via a unitary transformation of the initial Hamiltonian $\bar{\mathrm{H}}(0) = \mathrm{H}$

$$\bar{\mathrm{H}}(\alpha) = \mathrm{U}(\alpha)\mathrm{H}\mathrm{U}^\dagger(\alpha) \stackrel{\mathrm{2B}}{=} \mathrm{T} + \mathrm{V_{SRG}}(\alpha)\,, \tag{6}$$

where all α-dependent contributions have been absorbed in the renormalized interaction $\mathrm{V_{SRG}}(\alpha)$.

Again, the choice of the generator $\eta(\alpha)$ is crucial. Whereas the UCOM transformation is based on a static generator, the generator of the SRG transformation changes dynamically during the flow evolution. A simple choice for the generator was suggested by Szpigel and Perry [13] and used by Bogner *et al.* [14]

$$\eta(\alpha) = [\mathrm{T_{int}}, \bar{\mathrm{H}}(\alpha)] = \frac{1}{2\mu}[\mathbf{q}^2, \bar{\mathrm{H}}(\alpha)]\,, \tag{7}$$

which aims to diagonalize the two-body Hamiltonian $\bar{\mathrm{H}}(\alpha)$ in a basis of eigenstates of both p_r^2 and $\mathbf{L}^2$. Hence, in a partial-wave momentum-space basis $|q\,(LS)J\,T\rangle$ this generator drives the matrix elements towards a band-diagonal structure with respect to (q, q') and (L, L'). The flow equation (5) can be easily solved in this partial-wave momentum-representation yielding momentum space matrix elements of the evolved Hamiltonian.

Already on the formal level, we can relate the SRG scheme to the UCOM transformation. Let us assume a realistic NN interaction given in an operator representation similar to the Argonne V18 potential. The most relevant components for this consideration are the central and the tensor part of the interaction. If we formulate the initial Hamiltonian with this type of interaction and evaluate the initial generator $\eta(0)$ via the commutator relation (7) we easily obtain [12]

$$-\mathrm{i}\eta(0) = \frac{1}{2}\big[\mathrm{q}_r S(\mathrm{r}) + S(\mathrm{r})\mathrm{q}_r\big] + \frac{3}{2}\Theta(\mathrm{r})\big[(\boldsymbol{\sigma}_1\cdot\mathbf{q}_\Omega)(\boldsymbol{\sigma}_2\cdot\mathbf{r}) + (\mathbf{r}\leftrightarrow\mathbf{q}_\Omega)\big]\ . \tag{8}$$

This corresponds exactly to the structure of the central and tensor generators that were constructed in the UCOM approach based on physical considerations on the structure of short-range correlations. Both approaches address the same physics of short-range correlations. We utilize this connection to derive correlations funcitons in the UCOM framework, which correspond to the full SRG evolution up to a given flow parameter α.

2.3. *Three-body interactions*

So far, we have evaluated both unitary transformations, UCOM and SRG, in two-body space discarding induced interactions beyond the two-body level. When formulating the transformations in a general A-body space, one inevitably generates three-body, four-body, and higher-order interactions even if the initial Hamiltonian only contains a two-body force. Formally, we may write the transformed Hamiltonian in A-body space in terms of a cluster expansion

$$\begin{aligned}\widetilde{\mathrm{H}} &= \mathrm{C}^\dagger(\mathrm{T}+\mathrm{V_{NN}}+\mathrm{V_{3N}})\mathrm{C}\\ &= \widetilde{\mathrm{T}}^{[1]} + (\widetilde{\mathrm{T}}^{[2]} + \widetilde{\mathrm{V}}^{[2]}_{\mathrm{NN}}) + (\widetilde{\mathrm{T}}^{[3]} + \widetilde{\mathrm{V}}^{[3]}_{\mathrm{NN}} + \widetilde{\mathrm{V}}^{[3]}_{\mathrm{3N}}) + \cdots\\ &= \mathrm{T} + \mathrm{V_{UCOM}} + \mathrm{V}^{[3]}_{\mathrm{UCOM}} + \cdots\ ,\end{aligned} \tag{9}$$

where we have used the UCOM notation and assumed an initial Hamiltonian containing a two- and three-nucleon force. In addition to the tamed two-body interaction $\mathrm{V_{UCOM}}$ a three-body contribution $\mathrm{V}^{[3]}_{\mathrm{UCOM}}$ is generated. It contains induced three-body terms originating from the transformed kinetic energy, from the transformed two-body interaction, and from the transformed three-body interaction. Ideally the full three-body interaction—and possibly even higher-order contributions—would be taken into account when solving the many-body problem. Although the induced three-body contributions are formally well defined, their inclusion in an actual many-body calculation is a challenging task. The solution of the many-body problem would simplify tremendously if the effect of the three-body contributions could be reduced, i.e., if one could choose the unitary transformation such that the different three-body contributions, most notably the genuine three-body interaction $\mathrm{V}^{[3]}_{\mathrm{3N}}$ which is generally attractive and the induce three-body terms $\mathrm{T}^{[3]} + \mathrm{V}^{[3]}_{\mathrm{NN}}$ which are repulsive, cancel eachother.

Evidence that this is possible is provided by no-core shell model calculations in few-body systems [15] using the two-body part of the unitarily transformed interactions only. If all contributions were included, then the energy spectrum of the transformed and the initial Hamiltonian would be identical because of unitarity. If we can find a transformation that reproduces the energy

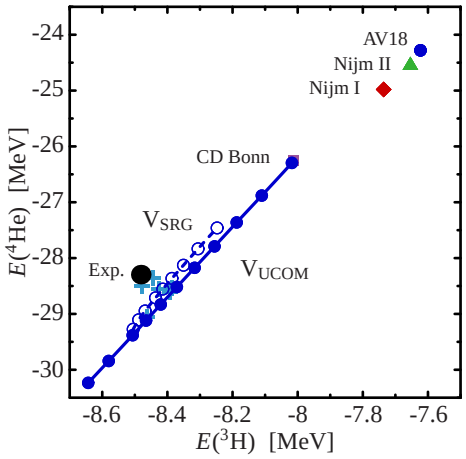

Fig. 2. Binding energies of ^{3}H and ^{4}He obtained in the no-core shell model [15] for different V_{UCOM} (full circles) and V_{SRG} (open circles) two-body interactions derived from the Argonne V18 potential. The labelled symbols in the upper part correspond to calculations with 'bare' interactions, the crosses around the experimental point indicate results for different two- plus three-body interactions [16].

eigenvalues of the initial Hamiltonian using only the two-body part of the transformed Hamiltonian, then the omitted higher-order terms must have vanishing contributions to the energy (not necessarily to the states).

This is illustrated in Fig. 2, where the ground state energies of ^{3}H and ^{4}He are shown for different 'bare' potentials and the 'tamed' potentials obtained in the UCOM and the SRG framework. As function of the range I_ϑ of the tensor correlation functions and of value α of the final flow parameter, respectively, the calculations with the transformed potentials span the Tjon line. For specific values of the parameter, the two-body potentials yield binding energies comparable to the experimental values and to results with conventional two- plus three-body interactions. Thus it is possible to choose a transformation for the which effectively minimizes the impact of higher-order interactions [17].

3. Importance Truncated No-Core Shell Model

These tamed interactions are the ideal input for different many-body approaches, ranging from the no-core shell model to Hartree-Fock based methods. Previously, we have shown that self-bound nuclei are obtained already on the level of Hartree-Fock [18], although long-range correlations cannot be described. Their inclusion via low-order many-body perturbation theory [18] or RPA ring-summations [19] leads to binding energies which are in agreement with experiment throughout the whole nuclear chart. This shows that the minimization of three-body contributions to the energy in the case of UCOM still works for heavier nuclei.

Here we discuss a scheme to extend the range of the no-core shell model to nuclei well beyond the p-shell [20]. The limiting factor for full no-core shell model calculations is the dimension of the model space, which grows dramatically with particle number and maximum excitation level $N_{\max}\hbar\Omega$. Therefore, converged no-core shell model calculations are presently limited to the p-shell. Most of the basis states included in these model spaces are irrelevant for the expansion of any particular eigenstate, i.e. their amplitudes are zero or extremely small. If one would exclude

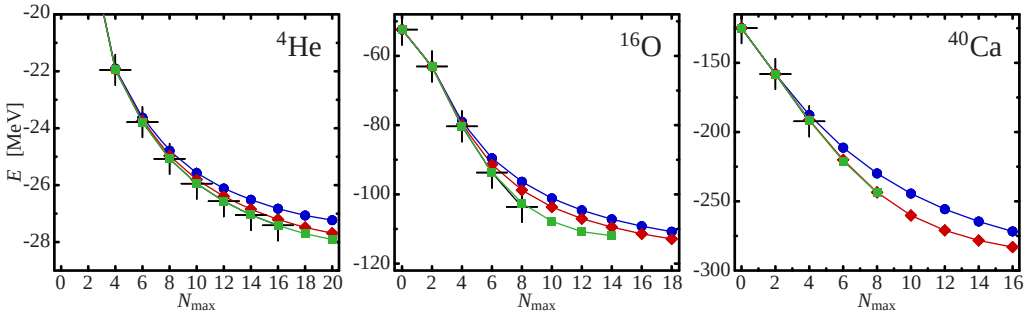

Fig. 3. Importance truncated no-core shell model calculations for ^{4}He, ^{16}O, and ^{40}Ca for an oscillator frequency $\hbar\Omega = 20$ MeV using the V_{UCOM} interaction fixed in the three- and four-body system. Shown are exact no-core shell model results (+) and results for an importance truncated model-space with up to 2p2h (●), 3p3h (♦), and 4p4h (■) excitations [20].

those irrelevant basis states from the outset, then the dimension of the eigenvalue problem could be reduced to a tractable size. A quantitative *a priori* measure for the imporantance of individual basis states can be constructed within many-body perturbation theory. Starting from a reference state $|\Psi_{\rm ref}\rangle$ which provides a zeroth-order approximation of the eigenstate we are interested in, we can estimate the contribution of other basis states $|\Phi_\nu\rangle$ via first order perturbation theory. This defines the importance measure $\kappa_\nu = -\langle\Phi_\nu|\,{\rm H}'\,|\Psi_{\rm ref}\rangle/(\epsilon_\nu - \epsilon_{\rm ref})$, where H′ describes the Hamiltonian associated with the perturbation and ϵ_ν and $\epsilon_{\rm ref}$ the unperturbed energies of the configurations. These quantities depend on the partitioning of the Hamiltonian and the nature of the reference state which can be a superposition of many shell-model basis states itself.

When starting from the single shell-model Slater determinant as reference state then the importance measure provides nonzero importance weights only for configurations containing up to 2p2h excitations. In order to access higher npnh-states, we embed the construction of the importance truncated space into an iterative scheme. In a first iteration all important basis states up to the 2p2h-level are constructed and the eigenvalue problem in this space is solved. Using the dominant components of the resulting eigenvector as a new reference state, we construct a new importance truncated space which then contains up 4p4h configurations. This iterative procedure can be repeated until the reference state does not change anymore. In the limit $\kappa_{\rm min} = 0$ this procedure generates the full no-core model space. In practice we will perform calculations for several values of $\kappa_{\rm min} \geq 0.00005$ and extrapolate the eigenvalues to $\kappa_{\rm min} = 0$.

Results for the ground-state energies of ^{4}He, ^{16}O, and ^{40}Ca as function of the model space size $N_{\rm max}$ obtained with V_{UCOM} are summarized in Fig. 3. For these calculations we have restricted ourselves to one iteration of the aforementioned cycle such that the model space is limited to 4p4h configurations. In comparison to full no-core shell model calculations performed with Antoine [21] (black crosses) the dramatic reduction of the model space dimension allows us to work in much larger $N_{\rm max}\hbar\Omega$ spaces.

This simple scheme has several advantages: Since we solve an eigenvalue problem in a restricted basis, we have direct access to the ground state as well as to excited states. The scheme can be viewed as a variational calculation using an adaptive trial state, the variational principle guarantees that we obtain an upper bound for the exact energy eigenvalues. Since we start from a complete $N_{\rm max}\hbar\Omega$-space, spurious center-of-mass excitations are absent and we have verified that the importance truncation does not generate them artificially. We directly obtain a shell model representation of the wavefunction which can easily be used to compute further ob-

servables. Apart from simple expectation values we are presently studying densities and form factors. The conceptual simplicity of the importance truncation scheme also allows for a variety of systematic extensions and improvements, e.g., through perturbative corrections for the excluded configurations. We have implemented corrections up to the 6p6h level using second-order perturbation theory. Similar importance selection techniques are being used in quantum chemistry in connection with configuration interaction methods [22]. In this context several simple correction methods, like multi-reference Davidson corrections which approximately restore size extensivity, have been developed and can be adopted for the importance truncated no-core shell model as well.

4. Conclusions

Nuclear theory presently experiences several exciting developments affecting all building blocks of our theoretical description of nuclei. The connection of nuclear interactions to the underlying theory of QCD is employed to derive consistent realistic interaction. These interactions can be used as basis for the construction of phase-shift equivalent tamed interactions, e.g. in the framework of the Unitary Correlation Operator Method or the Similarity Renormalization Group. They, in turn are a universal starting point for various approaches for treating the many-body problem. Also in this sector new approaches, like the importance truncated NCSM, will help to provide a consistent picture of nuclear structure for stable and exotic nuclei.

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