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Ab Initio Nuclear Structure Calculations with Transformed Realistic Interactions

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Abstract. We discuss three elements of modern *ab initio* nuclear structure theory with an emphasis on the role of correlations in the nuclear many-body problem. Starting from the QCD-motivated construction of a realistic nuclear interaction we review two methods to derive phase-shift equivalent tamed interactions, the Unitary Correlation Operator Method and the Similarity Renormalization Group. Eventually we use these interactions for *ab initio* calculations within the importance truncated no-core shell model.

1 Introduction

The rich physics of exotic nuclei poses an enormous challenge to modern nuclear structure theory. Motivated by a wealth of open questions, novel experimental possibilities, and new theoretical developments, the interest in predictive *ab initio* nuclear structure calculations for stable and exotic nuclei has intensified over the past years. The general goal for this line of research is to solve the nuclear many-body problem in a fully controlled way starting from realistic nuclear interactions. Of course, this problem has two components which pose enormous challenges in themselves: (a) the construction of realistic nuclear interactions and (b) the solution of the quantum many-body problem for a strongly correlated system of nucleons.

2 Modern Nuclear Interactions

The crucial ingredient for the description of the nucleus as a quantum many-body system of interacting nucleons is the interaction between these constituents. In this effective theory, the interaction encapsulates the unresolved dynamics of the underlying degrees of freedom — the quarks and gluons of Quantum Chromodynamics (QCD). It constitutes the link between the more fundamental theory of QCD and the effective description of the nucleus as a many-nucleon system. In principle, the interaction can be extracted from the explicit solution of the underlying theory. In practice, this route is widely used outside of nuclear physics, e.g. for the description of Helium liquids as an interacting system of inert Helium-atoms: The atom-atom interaction between neutral Helium atoms can be obtained from an *ab initio* solution of the electronic structure problem of the Helium dimer [1]. In nuclear physics, the underlying theory of low-energy QCD is so complicated, that this stringent approach was not feasible so far—only very recently first qualitative attempts have been made to extract a nucleon-nucleon interaction from lattice QCD calculations [2].

In the past, most *ab initio* nuclear structure calculations were based on realistic NN interactions constructed within a phenomenological framework, which typically uses a meson-exchange model supplemented by phenomenological short-range terms or cutoff functions. The

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parameters of these models are fitted such that the exact solutions of the two-body problem reproduce the experimental bound state (deuteron binding energy) and scattering data (scattering phase-shifts). All modern realistic interactions reproduce those two-body observables with high-precision.

Recently, chiral effective field theories have been used to establish and utilize the link between low-energy QCD and the nuclear interaction [3,4]. The long-range pion dynamics is included explicitly and the short-range physics is absorbed in contact terms. The chiral power expansion naturally leads to a consistent set of two-body, three-body, and higher-order interactions. In addition to the interactions, other operators, e.g. meson exchange current operators, can be derived in the same effective framework. Again the parameters, such as the low-energy constants associated with the contact terms, are chosen such that scattering phase-shifts and deuteron properties are reproduced. First applications of these chiral interactions in *ab initio* no-core shell model calculations of p-shell nuclei [5] demonstrate the potential of this concept.

3 Unitarily Transformed Realistic Interactions

Realistic interactions resulting from meson-exchange models or chiral effective field theory typically show rather slow convergence when used, e.g., in a no-core shell model (NCSM) calculation (cf. section 4). Model spaces of enormous size are required to obtain converged energies. This indicates that there are strong short-range correlations induced by the interaction, which play an important role for the structure and properties of the many-nucleon state. In the shell-model context, these correlations can only be described by a superposition of a large number of Slater determinants. This is illustrated in Fig. 1(a), where the dependence of the ground-state energy for ^{4}He on the size if the model space is depicted for the Argonne V18 (AV18) potential. With increasing $N_{\max}\hbar\Omega$, the maximum harmonic-oscillator excitation energy allowed in the many-body basis, the number of Slater determinants in the basis grows factorially. For $16\hbar\Omega$ the space already consists of a few million Slater determinants and the ground-state energy is still not converged, i.e., a superposition of millions of Slater determinants is still not sufficient to describe the correlated ground state of ^{4}He for the AV18 potential.

The dominant correlations responsible for the slow convergence can be traced back to certain components of the nucleon-nucleon interaction itself. Most important are short-range central correlations induced by the repulsive short-range part of the interaction and correlations induced by the strong tensor interaction. Already the ground state of the deuteron reveals these correlations: 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.

Unitary transformations can be used to tackle the problem of short-range correlations. The transformation has to suppress the components of the initial interaction that induce 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. 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 small 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. We will discuss two of these phase-shift conserving unitary transformations in the following sections.

3.1 Unitary Correlation Operator Method (UCOM)

The idea of the Unitary Correlation Operator Method (UCOM) [10,11] 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

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

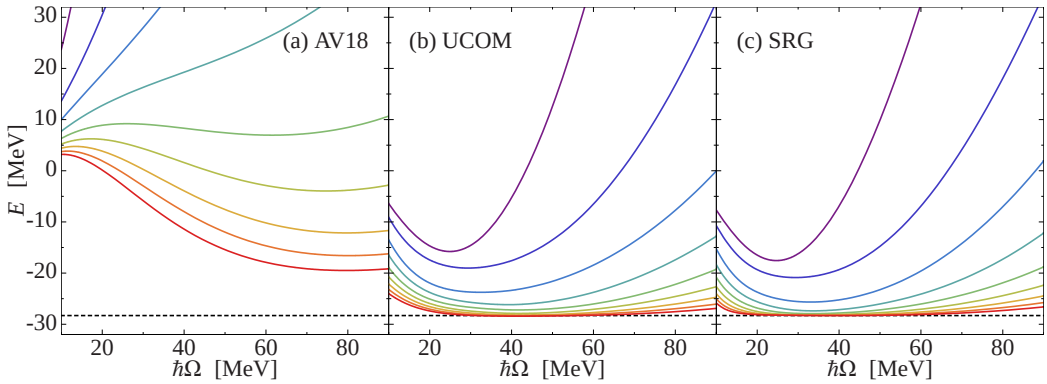

Fig. 1. Convergence of the ^{4}He ground-state energy within the no-core shell model (without Lee-Suzuki transformation) as function of the oscillator frequency $\hbar\Omega$. The curves correspond to different model space sizes from $0\hbar\Omega$ (topmost curves) to $16\hbar\Omega$ (bottom curves). The interactions used here are (a) the AV18 potential, (b) the UCOM-transformed interaction $V_{\rm UCOM}$, and (c) the SRG-evolved interaction $V_{\rm SRG}$ (see text).

Already the deuteron allows us to identify 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 nucleons are within the region of the short-range repulsion, then the transformation has to push them apart. This kind of distance-dependent shift is described by the unitary operator

$$C_r = \exp\Big[-{\rm i} \sum_{i<j} g_{r,ij} \Big] \qquad \text{with} \qquad g_r = \frac{1}{2}[s(r) q_r + q_r s(r)] \; , \tag{2}$$

where $q_r = \frac{1}{2}[\mathbf{q}\cdot(\mathbf{r}/r)+(\mathbf{r}/r)\cdot\mathbf{q}]$ 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 states with relative orbital angular momentum $L \pm 2$. This is achieved with the operator

$$C_\Omega = \exp\Big[-{\rm i} \sum_{i<j} g_{\Omega,ij} \Big] \qquad \text{with} \qquad g_\Omega = \frac{3}{2} \vartheta(r) \big[(\sigma_1 \cdot \mathbf{q}_\Omega)(\sigma_2 \cdot \mathbf{r}) + (\mathbf{r} \leftrightarrow \mathbf{q}_\Omega) \big] \; , \tag{3}$$

where $\mathbf{q}_\Omega = \mathbf{q} - \frac{\mathbf{r}}{r}\, q_r$ 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.

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

$$\widetilde{H} = C^\dagger \, H \, C = C^\dagger (T+V) C \stackrel{\rm 2B}{=} T + V_{\rm UCOM} \; , \tag{4}$$

which defines the tamed or correlated two-body interaction $V_{\rm UCOM}$. We will come back to the induced three-body contributions lateron. The fact that C is given in an explicit operator

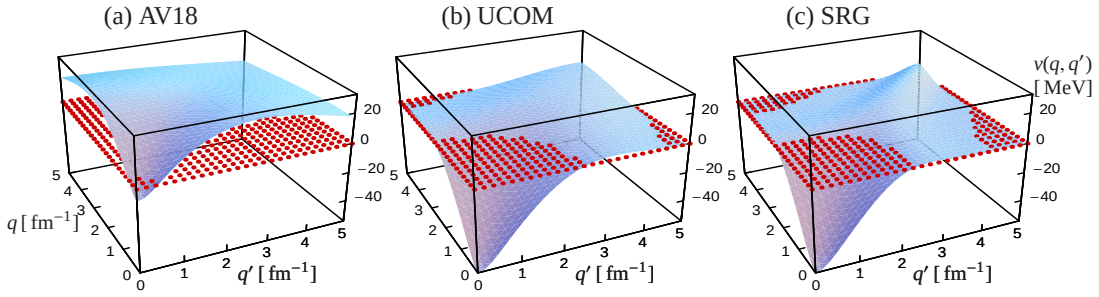

Fig. 2. Momentum-space matrix elements $v(q, q')$ in the $^3S_1$ partial wave for different interactions: (a) the AV18 potential, (b) the UCOM-transformed interaction V_{UCOM}, and (c) the SRG-evolved interaction V_{SRG} (see text).

representation is very convenient: It allows us to derive a closed operator form of the correlated interaction V_{UCOM}, which is necessary for many-body methods not based on simple orthogonal bases, like the Fermionic Molecular Dynamics approach [12]. Furthermore, operators of other observables, e.g. densities, form factors, transition amplitudes, and exchange currents, can be correlated consistently without additional effort.

For a first quantitative picture of the effect of the UCOM transformation we consider the matrix elements of V_{UCOM}. The V_{UCOM} used here and in the following is derived from the AV18 potential using central and tensor correlation functions discussed in detail in Ref. [20]. In Fig. 2 the momentum-space matrix elements of V_{UCOM} in the $^3S_1$ partial wave are compared to the matrix elements of the original AV18 interaction. The short-range central and tensor parts of the AV18 potential are responsible for the strong off-diagonal contributions in the matrix elements—the interaction connects states with low momentum q with states of high momentum q'. The coupling to high-lying states is another way of explaining the slow convergence of the NCSM. The UCOM transformation changes the matrix elements dramatically: The off-diagonal matrix elements are suppressed and the low-momentum, near-diagonal contributions are enhanced. Effectively the UCOM transformation acts like a pre-diagonalization.

This pre-diagonalization has a strong impact on the convergence properties of the transformed interaction. Figure 1(b) shows the ground-state energy of ^{4}He obtained with V_{UCOM} in the no-core shell model for different $N_{\max}\hbar\Omega$. In comparison to the initial AV18 interaction, the substantial improvement regarding the convergence behavior is evident. Based on the transformed interaction converged *ab initio* calculations become possible within tractable model spaces also for heavier systems.

3.2 Similarity Renormalization Group (SRG)

The Similarity Renormalization Group (SRG) as a second method using unitary transformations to tame the interaction starts from a completely different background. Unlike UCOM, where the physical mechanism responsible for correlations in the many-body state is used as a guiding principle, the SRG is based on the behavior of matrix elements and the idea of pre-diagonalization. In the formulation proposed by Wegner [13,14] 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. As function of a flow parameter α, the evolution of the Hamiltonian is described by the flow equation [15]

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

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

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

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

The choice of the generator $\eta(\alpha)$ is essential. 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 [16] and used by Bogner *et al.* [17]

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

which aims to diagonalize the two-body Hamiltonian $\bar{H}(\alpha)$ 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 matrix elements of the evolved Hamiltonian.

An example for momentum-space matrix elements resulting from the flow evolution starting with the AV18 potential is shown in Fig. 2(c). The flow parameter has been chosen such that the resulting two-body interaction reproduces the ^{4}He binding energy in an exact NCSM calculation (cf. Sec. 3.3). As in the case of the UCOM transformation, the SRG evolution suppresses the off-diagonal matrix elements and leads to a tamed interaction with matrix elements concentrated along the diagonal and in the low-momentum region. The convergence properties of the SRG evolved interaction, e.g. for the ground state of ^{4}He as depicted in Fig. 1(c), are very similar to those observed for the UCOM transformed interaction.

The relation between the SRG scheme to the UCOM transformation can also be illustrated on a formal level. 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 [15]

$$-\mathrm{i}\eta(0) = \frac{1}{2}\big[q_r S(r) + S(r) q_r\big] + \frac{3}{2}\Theta(r)\big[(\sigma_1 \cdot \mathbf{q}_\Omega)(\sigma_2 \cdot \mathbf{r}) + (\mathbf{r} \leftrightarrow \mathbf{q}_\Omega)\big] \;. \tag{8}$$

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 functions in the UCOM framework, which correspond to the full SRG evolution up to a given flow parameter α.

3.3 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

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

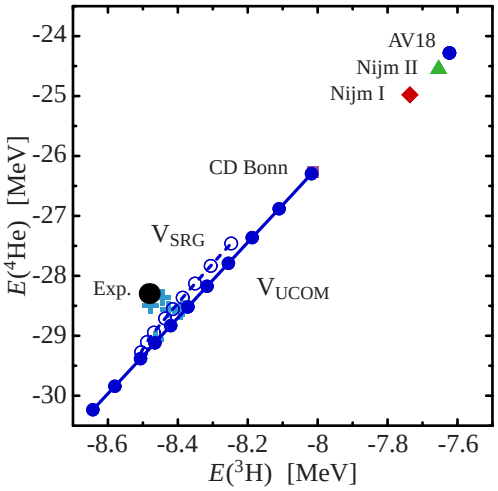

Fig. 3. Binding energies of ^{3}H and ^{4}He obtained in the NCSM [18] for different $V_{\rm UCOM}$ (full circles) and $V_{\rm SRG}$ (open circles) two-body interactions derived from the Argonne V18 potential. The labelled symbols in the upper part correspond to calculations with standard interactions, the crosses around the experimental point indicate results for different two- plus three-body interactions [19].

where we have used the UCOM notation. In addition to the two-body interaction $V_{\rm UCOM}$ a three-body contribution $V^{[3]}_{\rm UCOM}$ 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 transformed three-body interaction $\widetilde{V}^{[3]}_{\rm 3N}$ which is generally attractive and the induce three-body terms $\widetilde{T}^{[3]}+\widetilde{V}^{[3]}_{\rm NN}$ which are repulsive cancel each other.

Evidence that this is possible is provided by NCSM calculations [18] 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 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. 3, where the ground state energies of ^{3}H and ^{4}He are shown for different initial and transformed potentials obtained in the UCOM and the SRG framework. As function of the range of the tensor correlation functions and of value α of the final flow parameter, resp., 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 which effectively minimizes the impact of higher-order interactions [20]—the corresponding interactions $V_{\rm UCOM}$ and $V_{\rm SRG}$ were used in Figs. 1 and 2.

4 Advanced Many-Body Methods

The UCOM or SRG-transformed interactions are the ideal starting point for different many-body approaches, ranging from the NCSM to Hartree-Fock based methods. Previously, we have

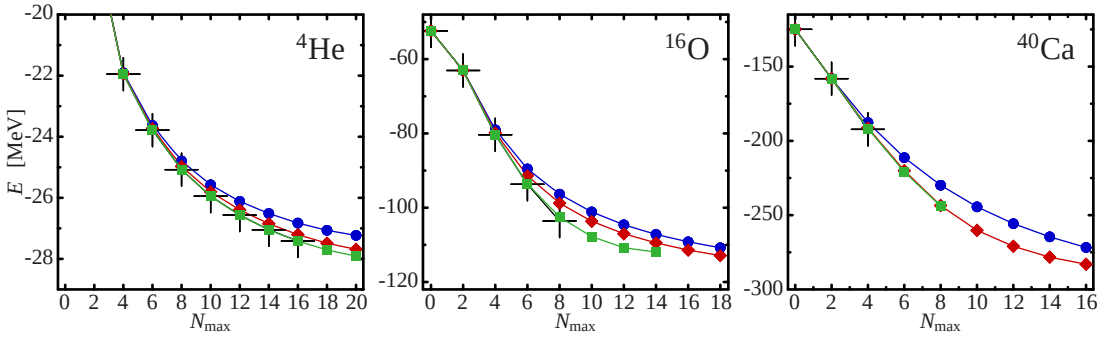

Fig. 4. Importance truncated no-core shell model calculations for ^{4}He, ^{16}O, and ^{40}Ca for an oscillator frequency $\hbar\Omega = 20$ MeV using the V_{UCOM} interaction fixed in the three- and four-body system. Shown are exact no-core shell model results (+) and results for an importance truncated model-space with up to 2p2h (disk), 3p3h (diamond), and 4p4h (square) excitations [22].

shown that self-bound nuclei are obtained already on the level of Hartree-Fock [21], although long-range correlations cannot be described. Their inclusion via low-order many-body perturbation theory [21] 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 NCSM to nuclei well beyond the p-shell [22]. The limiting factor for full NCSM calculations is the dimension of the model space, which grows factorially with particle number and maximum excitation level $N_{\max}\hbar\Omega$. Therefore, converged NCSM 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 selected eigenstate, i.e. their amplitudes are zero or extremely small. If one could exclude those irrelevant basis states from the outset, then the dimension of the eigenvalue problem would be reduced to a tractable size. A quantitative *a priori* measure for the importance of individual basis states can be constructed within many-body perturbation theory. Starting from a reference state $|\Psi_{\mathrm{ref}}\rangle$ 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 $\kappa_\nu = -\langle\Phi_\nu| H' |\Psi_{\mathrm{ref}}\rangle/(\epsilon_\nu - \epsilon_{\mathrm{ref}})$, where H' describes the Hamiltonian associated with the perturbation and ϵ_ν and ϵ_{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 the importance measure provides nonzero importance weights only for configurations containing up to 2p2h excitations. In order to access higher $np$$n$h-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 $\kappa_{\min} = 0$ this procedure generates the full no-core model space. In practice we will perform calculations for several values of $\kappa_{\min} \geq 5 \times 10^{-5}$ and extrapolate the eigenvalues to $\kappa_{\min} = 0$.

Results for the ground-state energies of ^{4}He, ^{16}O, and ^{40}Ca as function of the model space size $N_{\max}$ obtained with V_{UCOM} are summarized in Fig. 4. 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 the shell-model code ANTOINE [23] (black crosses) the dramatic reduction of the model space dimension allows us to work in much larger $N_{\max}\hbar\Omega$ 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 $N_{\max}\hbar\Omega$-space, intrinsic and center-of-mass motion are decoupled, 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 observables. 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.

5 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 interactions. 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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