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Ab initio No-Core Shell Model —Recent results and future prospects

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Abstract. The *ab initio* No-Core Shell Model (NCSM) adopts an intrinsic Hamiltonian for all nucleons in the nucleus. Realistic two-nucleon and tri-nucleon interactions are incorporated. From this Hamiltonian, an Hermitian effective Hamiltonian is derived for a finite basis space conserving all the symmetries of the initial Hamiltonian. The resulting finite sparse matrix problem is solved by diagonalization on parallel computers. Applications range from light nuclei to multiquark systems and, recently, to similar problems in quantum field theory. We present this approach with a sample of recent results.

PACS. 21.60.Cs Shell model – 23.20.-g Electromagnetic transitions – 23.20.Js Multipole matrix elements

1 Introduction

In the *ab initio* No-Core Shell Model (NCSM), we define an Intrinsic "bare" Hamiltonian to include a realistic nucleon-nucleon (NN) interaction and, in some cases, include a theoretical tri-nucleon (NNN) interaction. We utilize an NN interaction model that describes the NN data to high precision. This can be phenomenologically inspired or based on chiral field theory. These interactions may feature charge-symmetry breaking, may be non-local, and may be strongly repulsive at short distances. Recently obtained NN potentials from inverse scattering theory are also investigated and applied to light p-shell nuclei. The NNN interactions are taken from either meson-exchange theory or chiral field theory.

In order to accommodate the strong short-range correlations, we adopt an effective Hamiltonian approach, outlined below, in which a 2-body or 3-body cluster subsystem of the full A-body problem is solved exactly. From the exact solutions of the cluster subsystem, an effective Hamiltonian is evaluated in a model space appropriate to the no-core many-body application at hand. The full Hamiltonian is then approximated as a proper superposition of these cluster effective Hamiltonians and the no-core many-body problem is then solved in the chosen basis space [1]. The effective Hamiltonian and its eigensolutions respect the symmetries of the underlying NN and NNN interactions.

In this work, we indicate the utility of the *ab initio* NCSM for solving quantum many-body problems in other fields of physics. This utility is manifest when a limited number of fermions and/or bosons represents well the system of interest or a useful approximation to it. Specific references are made to multi-quark plus multi-antiquark systems and Hamiltonian formulations of quantum field theory. Indeed, initial applications to these systems have been published.

2 Ab initio No-Core Shell-Model

The method involves a similarity transformation of the "bare" Hamiltonian to derive an effective Hamiltonian for

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a finite model space based on realistic NN and NNN interactions [2,3,4,5,6,7,8]. Diagonalization and the evaluation of observables from effective operators created with the same transformations are carried out on high-performance parallel computers.

For pedagogical purposes, we outline the *ab initio* NCSM approach with NN interactions alone and point the reader to the literature for the extensions to include NNN interactions. Note that another paper in these proceedings addresses results with NNN interactions in more detail [9]. We begin with the purely intrinsic Hamiltonian for the A-nucleon system, *i.e.*,

$$H_A = T_{\rm rel} + \mathcal{V} = \frac{1}{A}\sum_{i<j}^{A}\frac{(\boldsymbol{p}_i - \boldsymbol{p}_j)^2}{2m} + \sum_{i<j=1}^{A} V_{\rm N}(ij)\ , \quad (1)$$

where m is the nucleon mass and $V_{\rm N}(ij)$, the NN interaction, with both strong and electromagnetic components. Note the absence of a phenomenological single-particle (sp) potential. We may use either coordinate-space NN potentials, such as the Argonne potentials [10] or momentum-space dependent NN potentials, such as the CD-Bonn [11].

Next, we add the center-of-mass HO Hamiltonian to the Hamiltonian (1) $H_{\rm CM} = T_{\rm CM} + U_{\rm CM}$, where $U_{\rm CM} = \frac{1}{2}Am\Omega^2\boldsymbol{R}^2$, $\boldsymbol{R} = \frac{1}{A}\sum_{i=1}^{A}\boldsymbol{r}_i$. At convergence, the added $H_{\rm CM}$ term has no influence on the intrinsic properties. However, when we introduce our cluster approximation below, the added $H_{\rm CM}$ term facilitates convergence to exact results with increasing basis size. The modified Hamiltonian, with a pseudo-dependence on the HO frequency Ω, can be cast into the form

$$H_A^\Omega = H_A + H_{\rm CM} = \sum_{i=1}^{A}\left[\frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2}m\Omega^2\boldsymbol{r}_i^2\right] + \sum_{i<j=1}^{A}\left[V_{\rm N}(ij) - \frac{m\Omega^2}{2A}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2\right]\ . \quad (2)$$

Next, we introduce a unitary transformation, which is designed to accommodate the short-range two-body correlations in a nucleus, by choosing an antihermitian operator S, acting only on intrinsic coordinates, such that

$$\mathcal{H} = e^{-S}H_A^\Omega e^{S}\ . \quad (3)$$

In our approach, S is determined by the requirements that $\mathcal{H}$ and H_A^Ω have the same symmetries and eigenspectra over the subspace $\mathcal{K}$ of the full Hilbert space. In general, both S and the transformed Hamiltonian are A-body operators. Our simplest, non-trivial approximation to $\mathcal{H}$ is to develop a two-body ($a = 2$) effective Hamiltonian, where the upper bound of the summations "A" is replaced by "a", but the coefficients remain unchanged. The next improvement is to develop a three-body effective Hamiltonian, ($a = 3$). This approach consists then of an approximation to a particular level of clustering with $a \le A$,

$$\mathcal{H} = \mathcal{H}^{(1)} + \mathcal{H}^{(a)} = \sum_{i=1}^{A} h_i + \frac{\binom{A}{2}}{\binom{A}{a}\binom{a}{2}}\sum_{i_1<i_2<\ldots<i_a}^{A}\tilde{V}_{i_1 i_2 \ldots i_a}\ , \quad (4)$$

with

$$\tilde{V}_{12\ldots a} = e^{-S^{(a)}}H_a^\Omega e^{S^{(a)}} - \sum_{i=1}^{a} h_i\ , \quad (5)$$

and $S^{(a)}$ is an a-body operator; $H_a^\Omega = h_1 + h_2 + h_3 + \ldots + h_a + V_a$, and $V_a = \sum_{i<j}^{a} V_{ij}$. Note that there is no sum over "a" in eq. (4). Also, we adopt the HO basis states that are eigenstates of the one-body Hamiltonian $\sum_{i=1}^{A} h_i$.

If the full Hilbert space is divided into a finite model space ("P-space") and a complementary infinite space ("Q-space"), using the projectors P and Q with $P+Q = 1$, it is possible to determine the transformation operator S_a from the decoupling condition

$$Q_a e^{-S^{(a)}}H_a^\Omega e^{S^{(a)}}P_a = 0\ , \quad (6)$$

and the simultaneous restrictions $P_a S^{(a)} P_a = Q_a S^{(a)} Q_a = 0$. Note that a-nucleon-state projectors (P_a, Q_a) appear in eq. (6). Their definitions follow from the definitions of the A-nucleon projectors P, Q.

We note that in the limit $a \to A$, we obtain the exact solutions for d_P states of the full problem for any finite basis space, with flexibility for choice of physical states subject to certain conditions [12].

Note that this approach has a significant residual freedom. There is an arbitrary residual P_a-space unitary transformation that leaves the a-cluster properties invariant. There is a similar freedom for the Q_a-space. Of course, the A-body results are not invariant under this residual transformation. An effort is underway to exploit this residual freedom to accelerate convergence in practical applications.

The model space, P_2, is defined by $N_{\rm m}$ via the maximal number of allowed HO quanta of the A-nucleon basis states, $N_{\rm M}$, using the condition that the sum of the nucleons' $2n + l \le N_{\rm m} + N_{\rm spsmin} = N_{\rm M}$, where $N_{\rm spsmin}$ denotes the minimal possible HO quanta of the spectators, *i.e.*, nucleons not affected by the interaction process. For example, ^{10}B, $N_{\rm spsmin} = 4$ as there are 6 nucleons in the $0p$-shell in the lowest HO configuration and, *e.g.*, $N_{\rm m} = 2 + N_{\rm max}$, where $N_{\rm max}$ represents the maximum HO quanta of the many-body excitation above the unperturbed ground-state configuration. For ^{10}B, in our nomenclature, $N_{\rm M} = 12$, $N_{\rm m} = 8$ for an $N_{\rm max} = 6$ or "$6\hbar\Omega$" calculation.

On account of our cluster approximation, a dependence of our results on $N_{\rm max}$ (or equivalently, on $N_{\rm m}$ or on $N_{\rm M}$) and on Ω arises. The residual $N_{\rm max}$ and Ω dependences can be used to infer the uncertainty in our results arising from effects associated with increasing a.

We input the effective Hamiltonian, now consisting of a relative 2-body operator and the pure $H_{\rm CM}$ term introduced earlier, into an m-scheme Lanczos diagonalization process to obtain the P-space eigenvalues and eigenvectors. At this stage we also add the term $H_{\rm CM}$ again with

a large positive coefficient (constrained via Lagrange multiplier) to separate the physically interesting states with $0s$ CM motion from those with excited CM motion. All observables that are expressible as functions of relative coordinates, such as the rms radius and radial densities, are then evaluated free of CM motion effects.

Note that all observables require the same transformation as implemented for the Hamiltonian. We obtain small effects on long range operators such as the rms radius operator and the $B(E2)$ operator when we transform them to P-space effective operators at the $a = 2$ cluster level [1,13]. On the other hand, substantial renormalization was observed for the kinetic energy operator when using the $a = 2$ transformation to evaluate its expectation value [14].

Recent applications include:

a) spectra and transition rates in p-shell nuclei;
b) comparisons between NCSM and Hartree-Fock [15];
c) di-neutron correlations in the ^{6}He halo nucleus [16];
d) neutrino cross sections on ^{12}C [17];
e) using inverse scattering theory plus NCSM to obtain novel NN interactions [18];
f) spectra of ^{16}C and ^{16}O [19];
g) spectroscopy of the $A = 47$–49 nuclei [20,21];
h) statistical properties of nuclei based on NCSM and approximations thereto [22];
i) exotic multiple quark systems [23];
j) plus others in quantum field theory that will not be discussed due to time limitations.

Let us survey some of these applications and rely on labels and captions to convey key information.

The ground-state energy of ^{6}Li [18] as a function of $\hbar\Omega$ provides a gauge of the rate of convergence with increasing model space as illustrated in fig. 1. The flatter the curve and the more densely packed the curves become with increasing basis space, then, the closer we are to the converged result. Note that the JISP6 interaction has been adjusted through a phase equivalent transformation, so as to retain its excellent description of the NN data and to provide a better fit to the properties of the p-shell nuclei up through $A = 6$ [18].

A family of such potentials is now under development that extend the range of nuclei well-described while retaining NN phase shift equivalence and the deuteron properties. We use another member of this family, called JISP16, to display in fig. 2 an observable related to elastic electron scattering, the RMS point proton radius of ^{4}He. Each curve again represents the results in a fixed model space ranging over 0–14$\hbar\Omega$. The convergence with increasing model space, the tendency towards independence of the oscillator parameter, is good enough that by 8$\hbar\Omega$ the final result is obtained to within a few percent. While the convergence of the RMS is a demanding test of our approach, the results for ^{4}He should not be considered as typical. We expect that the convergence of the RMS neutron radius of a halo nucleus will be slower than for this tightly bound nucleus due to the fact that we work within an oscillator basis.

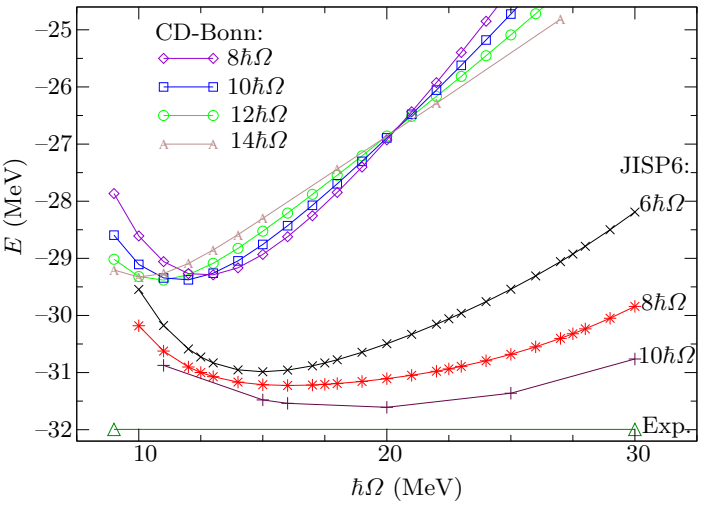

Fig. 1. Ground-state energy (MeV) of ^{6}Li with the CD-Bonn [11] and JISP6 [18] effective interactions in various basis spaces as a function of the oscillator parameter.

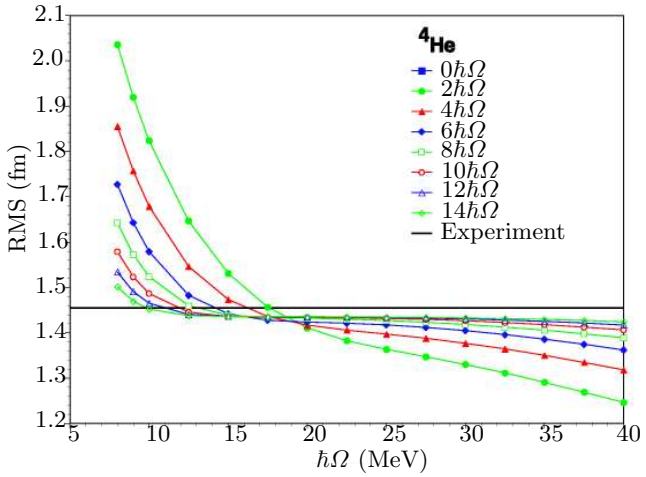

Fig. 2. Point proton root-mean-square (RMS) radius of ^{4}He with the JISP16 [18] effective interactions in various basis spaces as a function of the oscillator parameter.

The ground-state energies obtained in the *ab initio* NCSM often follow smooth trends as a function of both $\hbar\Omega$ and $N_{\max}$ as seen, for example, in fig. 1. We display the minima of such sequences of curves for ^{16}O in fig. 3 for four NN potentials. These minima also follow smooth trajectories and allow a good fit with a constant plus exponential function for each NN potential as shown. This extrapolation method has proven successful in lighter nuclei where results closer to convergence are used to test its accuracy. The obtained constants yield our predictions for the fully converged binding energies which are $-117(3)$, $-116(5)$, $-138(3)$, $-111(5)$ MeV for the CD-Bonn, AV8', INOY-3, N3LO potentials respectively. Our uncertainty in the last digit is indicated in parenthesis and is based on experience with different extrapolation strategies with these results. The results straddle the experiment (-127.619 MeV) and indicate the possible role of NNN potentials which are, in principle, different for each NN potential.

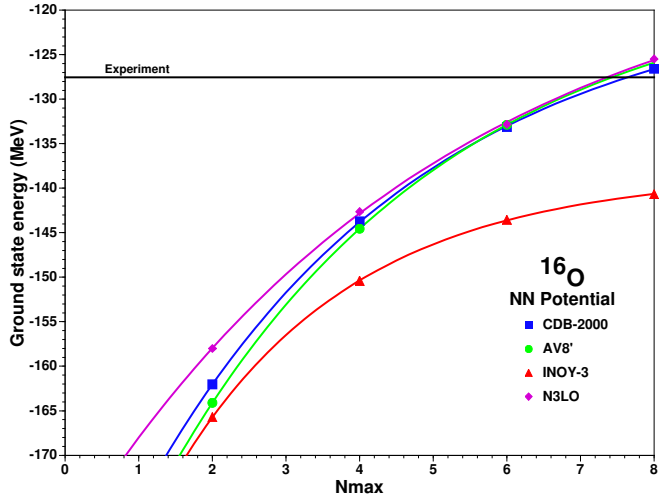

Fig. 3. Ground-state energy of ^{16}O [19] in the *ab initio* NCSM with 4 realistic NN potentials as a function of basis space size [11,24,25,26]. The points correspond to the minimum energy as a function of $\hbar\Omega$ at fixed $N_{\max}$. The smooth curves are constants plus exponentials fit to these results with $N_{\max} = 2$–8.

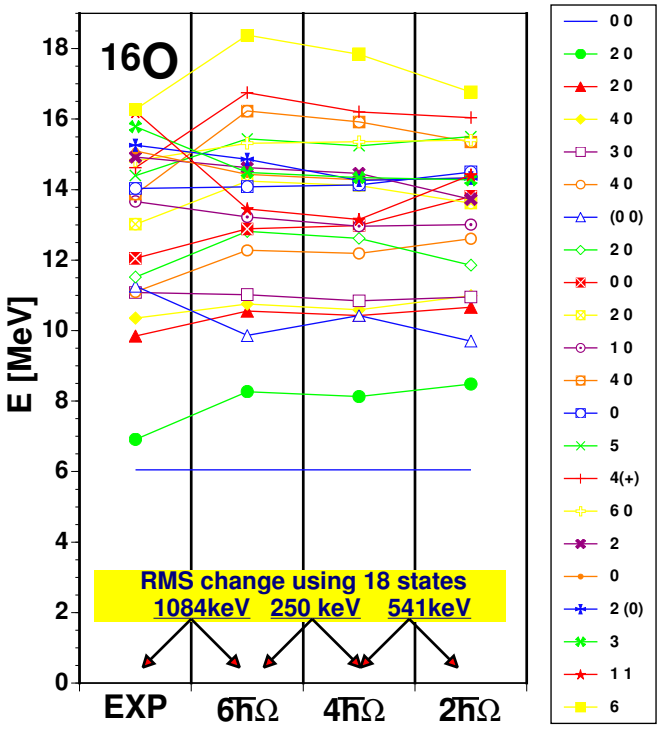

Fig. 4. Low-lying positive-parity ^{16}O states from the CD-Bonn interaction at the $a = 2$ cluster approximation in the NCSM with $\hbar\Omega = 15$ MeV. The spectra are aligned with the experimental first-excited 0^+ state.

The positive-parity excitation spectra of ^{16}O in fig. 4 show a favorable convergence trend when proceeding to larger basis spaces. In particular, we note that the rms difference between spectra in successive model spaces decreases significantly when progressing from the $2\hbar\Omega$ up through the $6\hbar\Omega$ model spaces. This trend suggests a converging spectra yet the rms differences from the experimental spectra are large (1.1 MeV) compared to the change in the last model space increase (0.25 MeV). From the sizable residual disparity with experiment, we conclude there is a need for genuine NNN potentials.

3 Phenomenological No-Core Shell Model

We now turn to heavier systems and select the ^{48}Ca region since the lightest nuclear candidate for neutrinoless double beta-decay is ^{48}Ca. Given the intense interest in this process as a method of inferring the Majorana mass of the neutrino or for indicating the presence of processes beyond the Standard Model, it is important that we focus considerable effort on this nucleus and its neighbors.

At present, computational limits prevent a sequence of multi-$\hbar\Omega$ basis space evaluations so we resort to small no-core basis spaces (0–1$\hbar\Omega$) and introduce phenomenological two-body terms to correct for the expected deficiencies. We use the name "*ab initio* NCSM" solely for results obtained within the framework outlined above. When we resort to phenomenological adjustments of the Hamiltonian, we will omit the label "*ab initio*" and simply refer to the results as obtained within the "NCSM". Even with the phenomenological adjustments, our results are obtained with a pure two-body Hamiltonian, *i.e.* without single particle energies, and in a no-core model space leading to significant differences from traditional shell-model calculations in valence spaces.

The specific forms we found adequate in fits to the low-lying the spectra of ^{48}Ca, ^{48}Sc and ^{48}Ti consist of finite-range central and tensor potentials as follows:

$$V(r) = V_0 e^{-(r/R)^2}/r^2 + V_1 e^{-(r/R)^2}/r^2 + V_t S_{12}/r^3\,, \quad (7)$$

where the isospin-dependent central strengths, V_T, are set at $V_0 = -14.40$ MeV fm^2 and $V_1 = -22.61$ MeV fm^2 with $R = 1.5$ fm, the tensor strength $V_t = -52.22$ MeV fm^3, and S_{12} is the conventional tensor operator.

Good spectra emerge [20,21] as well as good total binding energies shown in fig. 5 with the added terms.

The foremost deficiency of the CD-Bonn $H_{\rm eff}$ in these small model spaces is traced to insufficient splitting between the $0f_{7/2}$ and the $1p_{3/2}$ orbits as seen in the rightmost column of fig. 6. This is repaired well by the addition of the phenomenological two-body interaction terms. (Note that ^{47}Ca was not involved in our fitting procedures.) This defect appears to be a continuation of the insufficient spin-orbit splitting problem well-documented in a variety of light nuclei results. Hence, it is likely that the resolution of this problem will ultimately come from the addition of genuine NNN interactions.

4 Further applications of the ab initio No-Core Shell-Model

We have investigated the use of the *ab initio* NCSM to predict level densities for nuclei and to compare with simpler

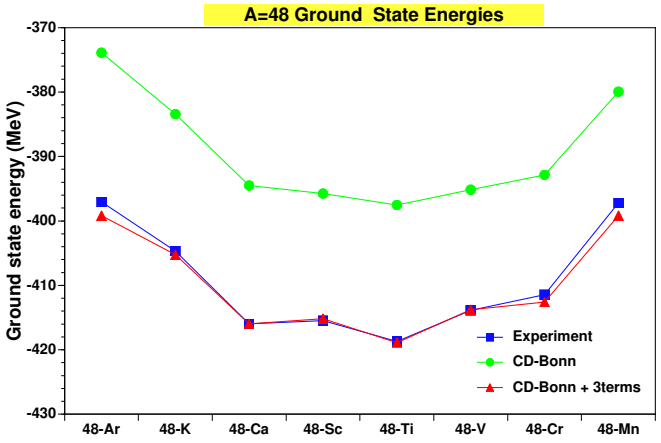

Fig. 5. Ground-state energies in MeV of $A = 48$ nuclei. At the extremes of the valley of stability, these experimental energies are determined by only systematics. The *ab initio* NCSM results labelled "CD-Bonn" are obtained with $H_{\rm eff}$ in the $1\hbar\Omega$ model space, $\hbar\Omega = 10$ MeV and isospin breaking in the P-space, as appropriate to ^{48}Ca. The same $H_{\rm eff}$ with an added Gaussian central $T = 0$ term, a similar central $T = 1$ term and a tensor force is used for the results labeled "CD-Bonn + 3 terms".

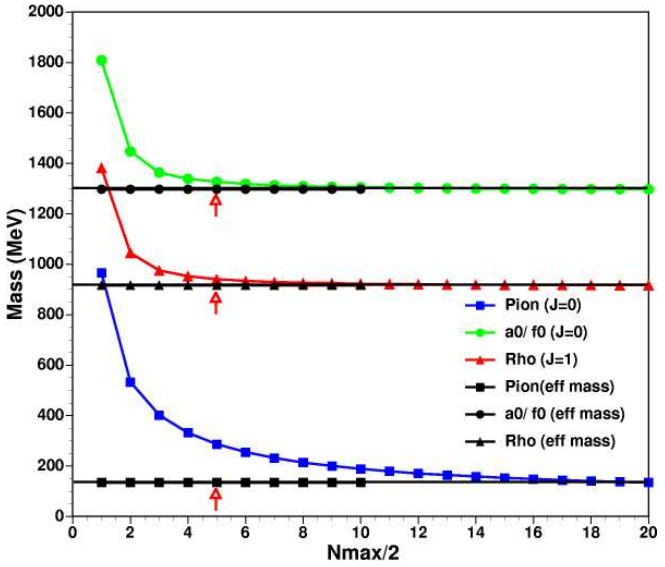

Fig. 7. Three low-lying meson masses as a function of $N_{\rm max}/2$. Both the bare Hamiltonian (points following curved trajectories) and the effective Hamiltonian (points following straight lines) are solved in an oscillator basis.

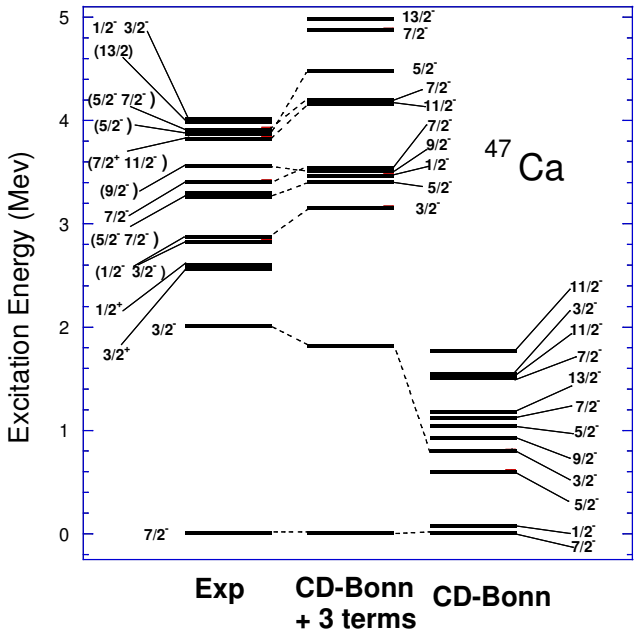

Fig. 6. Negative-parity spectra of ^{47}Ca obtained with the same Hamiltonians as for fig. 5.

methods [22], one of which we have developed specifically for no-core models. The initial results are very encouraging. We find that a mean-field treatment with the derived $H_{\rm eff}$ to generate the self-consistent single-particle spectrum [15], followed by statistical occupancy of those levels, can well-reproduce the *ab initio* NCSM results especially at higher excitation energies or higher temperatures. One subtlety, that we are currently studying, concerns the role of the spurious CM excitation which is absent in the NCSM but present in models based on single-particle spectra.

In order to provide a sense of the wide range of applications for the *ab initio* NCSM emerging in nuclear physics, we present in fig. 7 a constituent-quark model mass spectrum for three light mesons as a function of $N_{\rm max}/2$. The Hamiltonian consists of a potential derived from a relativistic wave equation treatment motivated by QCD and supplemented with traditional assumptions of massive constituent quarks [27]. It contains a term resembling one-gluon exchange and a term with behavior close to linear confinement.

One major goal of this effort is to predict masses for exotic multiquark systems with sufficient precision to guide experimental searches as we have demonstrated for all-charm tetraquarks [23]. For this reason, all the techniques of the *ab initio* NCSM are needed, including the effective Hamiltonian treatment, as seen by the slow convergence of the bare Hamiltonian mass spectra with increasing basis size. Note that the inclusion of the flavor degree of freedom here is analogous to our isospin treatment in the case of nucleons. However, the introduction of color represents a major additional degree of freedom as we seek to predict global color singlet states which are antisymmetric under that exchange of color, and which lie below breakup thresholds into known mesons and baryons.

Given the rapid progress of the *ab initio* NCSM in the last four years, one anticipates additional applications and extensions. It should have continuing impact on developing the nuclear many-body "standard model" including improvements in the NN and NNN interactions. It should contribute high-precision results for the determination of fundamental symmetries in nature such as nuclear double beta decay and the neutrino mass determination. Extensions to scattering theory and to the

structure of heavier nuclei are underway. Recently, applications to non-perturbative solutions of quantum field theory have appeared [28] and underscore the potential for cross-disciplinary applications.

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