Institute of Physics Publishing
doi:10.1088/1742-6596/20/1/012

Ab initio no-core shell model for light nuclei and other applications

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Abstract. The *ab initio* No-Core Shell Model (NCSM) begins with an intrinsic Hamiltonian for all nucleons in the nucleus. Realistic two-nucleon and tri-nucleon interactions are incorporated such as those recently developed from effective field theory and chiral perturbation theory. We then derive a finite basis-space dependent Hermitian effective Hamiltonian that conserves all the symmetries of the initial Hamiltonian. The resulting finite Hamiltonian matrix problem is solved by diagonalization on parallel computers. Applications range from light nuclei to multiquark systems and, recently, to quantum field theory including systems with bosons. We present this approach with a sample of recent results.

1. Introduction

It is a great pleasure to outline one of the present-day branches of nuclear theory that is firmly based on the pioneering works of both of our distinguished honorees - Professors Akito Arima and Igal Talmi. Among their many achievements, configuration mixing and the multi-particle harmonic oscillator representation are fundamental to our successes.

In the *ab initio* No-Core Shell Model (NCSM), we define an Intrinsic "bare" Hamiltonian to include a realistic nucleon-nucleon (NN) interaction and a theoretical tri-nucleon (NNN) interaction. The NN interaction model describes the NN data to high precision. The interactions may arise from any theoretical framework (meson exchange, effective field theory, chiral field theory, inverse scattering,...) and may have complicated features such as charge-symmetry breaking, non-locality, and strong repulsive at short distances, among others.

In order to accommodate strong short-range correlations, we adopt an effective Hamiltonian approach 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 A-body effective Hamiltonian is approximated as a superposition of these cluster effective Hamiltonians and the no-core many-body problem is solved in the chosen basis space [1]. The A-body 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. We refer to multi-quark plus antiquark systems and Hamiltonian formulations of quantum field theory where initial applications have appeared.

2. *Ab initio* theory of the nuclear shell model

The method involves a similarity transformation of the "bare" Hamiltonian to derive an effective Hamiltonian for a finite model space based on realistic NN and NNN interactions [2]. 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. We begin with the purely intrinsic Hamiltonian for the A-nucleon system, i.e.,

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

where m is the nucleon mass and $V_{\rm N}(ij)$, the NN interaction, with both strong and electromagnetic components. We may use either coordinate-space NN potentials, such as the Argonne potentials [3] or momentum-space dependent NN potentials, such as the CD-Bonn [4].

Next, we add to (1) the center-of-mass Harmonic Oscillator (HO) Hamiltonian $H_{\rm CM} = T_{\rm CM} + U_{\rm CM}$, where $U_{\rm CM} = \frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R} = \frac{1}{A}\sum_{i=1}^{A}\vec{r}_i$. 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 pseudo-dependence on the HO frequency Ω, can be cast as:

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

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

$$\mathcal{H} = e^{-S}H_A^{\Omega}e^{S}\ . \tag{3}$$

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. We then have an approximation at a fixed level of clustering, a, with $a \leq A$.

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

with

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

and $S^{(a)}$ is an a-body operator; $H_a^{\Omega} = h_1 + h_2 + h_3 + \ldots + h_a + V_a$, and $V_a = \sum_{i<j}^{a} V_{ij}$. We adopt the HO basis states that are eigenstates of the one-body Hamiltonian $\sum_{i=1}^{A} h_i$.

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 $P + Q = 1$. We determine the transformation operator S_a from the decoupling condition $Q_a e^{-S^{(a)}} H_a^{\Omega} e^{S^{(a)}} P_a = 0$ and the simultaneous restrictions $P_a S^{(a)} P_a = Q_a S^{(a)} Q_a = 0$. The a-nucleon-state projectors (P_a, Q_a) follow from the definitions of the A-nucleon projectors P, Q.

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 [5]. This approach has a significant residual freedom through an arbitrary residual P_a–space unitary transformation that leaves the a-cluster properties invariant. 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, $N_{\rm M}$, where the sum of the nucleons' $2n + l \leq N_{\rm m} + N_{\rm spsmin} = N_{\rm M}$, and where $N_{\rm spsmin}$ denotes the minimal possible HO quanta of the spectators. For ^{10}B, $N_{\rm M} = 12, N_{\rm m} = 8$ for an $N_{\rm max} = 6$ or "$6\hbar\Omega$" calculation. With 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 will infer the uncertainty in our results.

At this stage we also add the term H_{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. We diagonalize the effective Hamiltonian with an m-scheme Lanczos method to obtain the P-space eigenvalues and eigenvectors. All observables are then evaluated free of CM motion effects. In principle, all observables require the same transformation as implemented for the Hamiltonian. We obtain small renormalization 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, 6]. On the other hand, when a=2, substantial renormalization was observed for the kinetic energy operator [7]. and for higher momentum transfer observables [6].

Recent applications include:

(a) spectra and transition rates in p-shell nuclei;

(b) comparisons between NCSM and Hartree-Fock [8];

(c) di-neutron correlations in the ^{6}He halo nucleus [9];

(d) neutrino cross sections on ^{12}C [10];

(e) novel NN interactions using inverse scattering theory plus NCSM [11];

(e) spectra of ^{16}C and ^{16}O [12];

(f) spectroscopy of the $A = 47 - 49$ nuclei [13, 14];

(g) statistical properties of nuclei based on NCSM and approximations thereto [15];

(h) exotic multiple quark systems [16];

(i) plus others in quantum field theory that will not be discussed due to time limitations.

We first feature results with a soft and bare NN interaction, JISP16, that has been adjusted through phase equivalent transformations, so as to retain its excellent description of the NN data while fitting the properties of the p-shell nuclei up through $A = 16$ [11]. The ground and

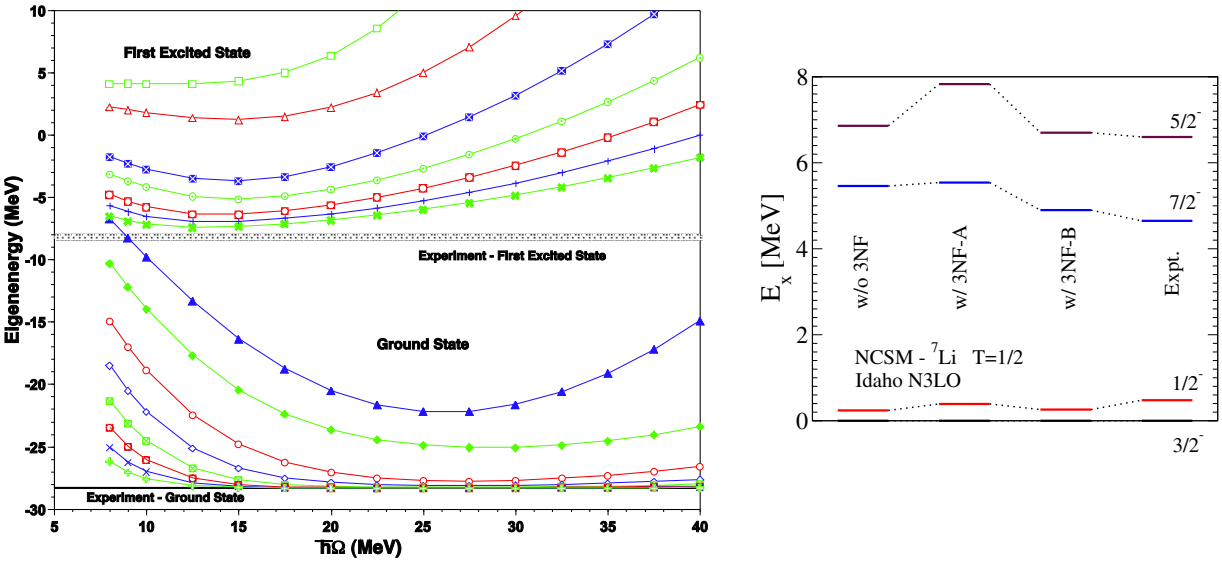

Figure 1. [Left panel] Ground and first excited states of ^{4}He with the JISP16 [11] bare interaction in basis spaces up to $N_{max} = 14$ as a function of HO energy. [Right panel] Low lying spectra of ^{7}Li with Idaho N3LO NN potential [18] alone and with two chiral NNN potentials[19].

first excited states of ^{4}He [11] as a function of $\hbar\Omega$ in Fig. 1 illustrate convergence with increasing model space. Flatter and more densely packed curves signal convergence with increasing N_{max}. We also find convergence for the ground state RMS radius while the RMS radius of the excited state shows divergence as one expects for a continuum state. Results obtained with H_{eff} for JISP16 (not shown) are more rapidly convergent than the bare H results but the energies do not systematically converge from above since the variational character is absent.

In the right panel of Fig. 1 we display recent results for ^{7}Li [17] obtained with NN and NNN potentials having their roots in QCD. Here, we use the a=3 cluster approximation in an 6 $\hbar\Omega$ model space at values of $\hbar\Omega$ where the ground state energy is minimized. Available NNN strength parameters are adjusted to fit the binding of the A=3 and A=4 systems and results with two such fits are shown. Simultaneous good descriptions of both binding and spectra of ^{7}Li emerge when chiral NNN interactions are included.

3. Modified no core shell model

We now turn to heavier systems near ^{48}Ca since it is the lightest nuclear candidate for neutrinoless double beta-decay. 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 these nuclei.

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 restrict our use of the name "*ab initio* NCSM" solely to 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 spectra of ^{48}Ca, ^{48}Sc and ^{48}Ti

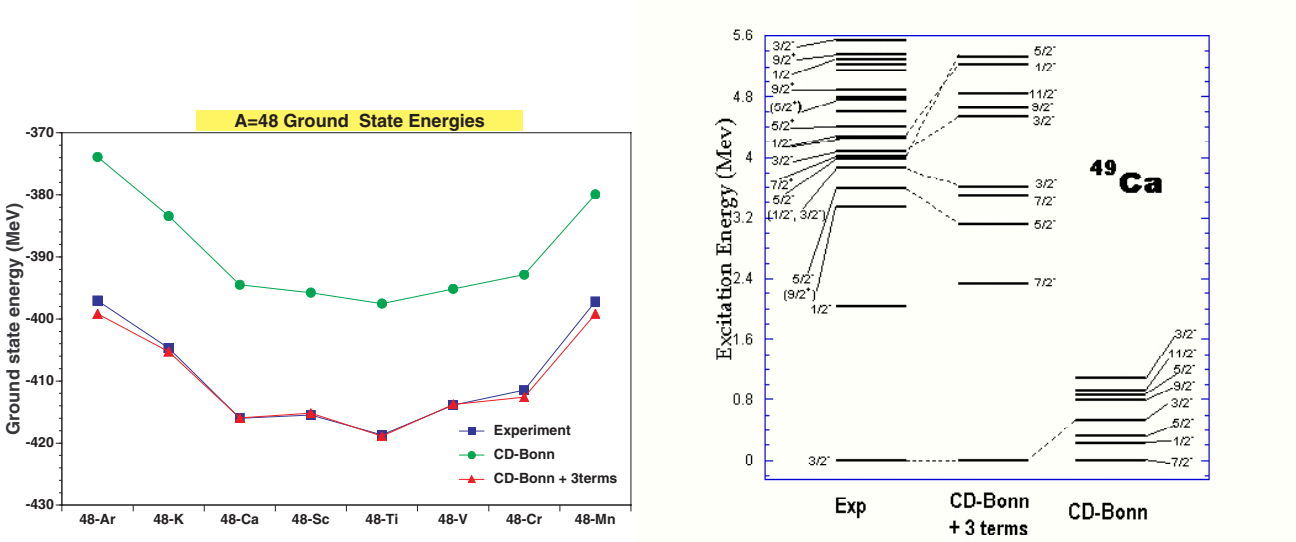

Figure 2. [Left panel] Ground state energies in MeV of $A = 48$ nuclei. At the extremes of the valley of stability, these experimental energies are determined by systematics. The *ab initio* NCSM results labelled "CD-Bonn" [4] are obtained with H_{eff} in the $1\hbar\Omega$ model space, $\hbar\Omega = 10\ MeV$ and isospin breaking in the P-space, as appropriate to ^{48}Ca. The same H_{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". [Right panel] Negative parity spectra of ^{49}Ca obtained with the same Hamiltonians as the left panel

consist of finite range central and tensor potentials as follows:

$$V(r) = V_0 e^{-(r/R)^2}/r^2 + V_1 e^{-(r/R)^2}/r^2 + V_t S_{12}/r^3 \tag{6}$$

where the isospin-dependent central strengths, V_T, are set at $V_0 = -14.40\ MeV \cdot fm^2$ and $V_1 = -22.61\ MeV \cdot fm^2$ with $R = 1.5\ fm$, the tensor strength $V_t = -52.22\ MeV \cdot fm^3$, and S_{12} is the conventional tensor operator. Good spectra emerge [13, 14] as well as good total binding energies shown in the left panel of Fig. 2 with the added terms.

The foremost deficiency of the CD-Bonn H_{eff} in these small model spaces is incorrect ordering of the $0f_{7/2}$ and the $1p_{3/2}$ orbits as seen on the far right of Fig. 2. This defect, reflecting the insufficient spin-orbit splitting well-documented in light nuclei, is repaired by the added phenomenological terms. Note that ^{49}Ca was not involved in our fitting procedures. It is likely that the resolution of this problem requires the addition of NNN interactions.

4. Applications of the *ab initio* no core shell model to field theory

We have investigated the use of the *ab initio* NCSM to predict level densities for nuclei and to compare with simpler methods [15], 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_{eff} to generate the self-consistent single-particle spectrum [8], 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 have calculated a constituent quark model mass spectrum for the light and heavy mass mesons as a function of N_{max}. 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 [21]. It contains a term resembling one-gluon exchange and a term with behavior close to linear confinement.

A 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 [16]. For this reason, all the techniques of the *ab initio* NCSM are needed, including the effective Hamiltonian treatment, due to a slow convergence of the bare Hamiltonian mass spectra with increasing basis size. The introduction of color represents a challenging 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 few 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 [20] and underscore the potential for cross-disciplinary applications.

This work was supported by the U. S. Department of Energy Grants DE-FG02-87ER40371, DE-F02-01ER41187, DE-FG02-00ER41132, and Contract W-7405-Eng-48, by the U.S. National Science Foundation, Grants PHY0070858, PHY0244389, PHY0071027, INT0070789, RFBR grants 02-02-17316 and 05-02-17429, and by Lawrence Livermore National Laboratory LDRD contract 00-ERD-028.

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