No-core shell model in an effective-field-theory framework

I. Stetcu, B.R. Barrett, and U. van Kolck
Department of Physics, University of Arizona, Tucson, Arizona 85721
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We present a new approach to the construction of effective interactions suitable for many-body calculations by means of the no-core shell model (NCSM). We consider an effective field theory (EFT) with only nucleon fields directly in the NCSM model spaces. In leading order, we obtain the strengths of the three contact terms from the condition that in each model space the experimental ground-state energies of ^{2}H, ^{3}H and ^{4}He be exactly reproduced. The first $(0^+;0)$ excited state of ^{4}He and the ground state of ^{6}Li are then obtained by means of NCSM calculations in several spaces and frequencies. After we remove the harmonic-oscillator frequency dependence, we predict for ^{4}He an energy level for the first $(0^+;0)$ excited state in remarkable agreement with the experimental value. The corresponding ^{6}Li binding energy is about 70% of the experimental value, consistent with the expansion parameter of the EFT.

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The microscopic description of quantum systems, from nuclei to atoms and molecules, is a very difficult task that often involves solving numerically the many-body Schrödinger equation in a restricted space. A longstanding challenge has been the construction of effective interactions within the finite model space where the many-body problem is solved [1]. In order to avoid uncontrolled approximations often invoked, we present a novel approach based on the general principles of effective field theory (EFT), which relates intimately the effective interactions (and, in general, effective operators describing interactions with external probes) with the model space.

The no-core shell model (NCSM) is a powerful many-body technique that provides the solution to the Schrödinger equation for A interacting nucleons in a restricted space [2]. The NCSM basis states are constructed using harmonic-oscillator (HO) wave functions. Starting from two-nucleon (NN) interactions that accurately fit the experimental phase shifts and deuteron properties, and theoretical three-nucleon (3N) forces adjusted to reproduce triton properties, one generally uses a unitary transformation approach to obtain effective interactions in a restricted model space, where an exact diagonalization in a many-body basis can be performed. This approach has been very successfully applied to the description of energy spectra of ^{4}He and light nuclei throughout the p shell [2, 3], and even beyond [4]. However, the results remain dependent on the details of the two- and three-body interactions used as input. Moreover, the method involves the "cluster approximation," which neglects higher-body correlations in a less controlled way. Finally, at the two-body-cluster level low-momentum observables, such as the quadrupole moment, are difficult to obtain using effective operators consistent with the interaction [5]. The description of low-momentum observables requires large model spaces, which makes the application of the method to heavy nuclei extremely challenging.

These problems can be mitigated if one formulates the problem as an EFT in a discrete basis. The basic idea underlying EFTs is that the restriction of a theory to a model space generates all interactions allowed by the theory's symmetries [6]. Since particle momenta are limited within the restricted space, one can treat short-distance interactions in a derivative expansion, similar to the multipole expansion in classical electrodynamics. The coefficients of this expansion carry information about the details of the short-range dynamics. In addition, these parameters depend on the size of the model space in such a way as to make the results for low-energy observables independent of the size of the space. Even in the absence of exact solutions from QCD, EFTs provide a modern understanding of the nuclear forces at low energies [7]. An EFT with pion fields can be constructed and generalizes chiral perturbation theory to nuclear systems, although its renormalization is still being explored [8]. At sufficiently low energies, a simpler EFT without explicit pions exists, and it has been shown to have a well-defined organizational principle ("power counting") [9], and give good results for ^{2}H [10], ^{3}H [11], and even the ground state of ^{4}He [12]. In leading order (LO), the pionless EFT has three parameters: two NN contact interactions that contribute to the NN $^3S_1$ and $^1S_0$ channels [9, 10], and one 3N contact interaction that appears in the 3N $S_{1/2}$ channel [11]. With trivial modifications, this EFT has also proved useful for atomic and molecular systems with large scattering lengths [13]. While continuum momentum-space calculations are considerably simplified in this EFT, they are still quite involved beyond the four-body system. First attempts have been made to derive bulk properties of matter using a spatial lattice [14], but the limit of applicability of the pionless theory with increasing density is at present unknown.

In this paper, we combine the virtues of the two approaches: we explore an implicit removal of the so-called excluded (or Q) space in the NCSM by using the EFT

principles (including power counting), thereby providing solutions of the EFT for heavier systems. The earlier successes of the standard shell model (an inert core plus a few valence nucleons) suggest that it might be interpretable as an EFT. For example, one hopes that EFT power counting might eventually explain why a good description of nuclear properties can be achieved using essentially one- and two-body terms in the Hamiltonian plus some A-dependence [15]. While some attempts to infuse EFT ideas into the shell model have been investigated in the past [16], we follow a different approach.

We start with the EFT Hamiltonian in the NCSM basis. The HO frequency, which we denote by ω, sets the spacing between HO levels and provides an infrared energy cutoff $\hbar\omega$ or, equivalently, a momentum cutoff $\lambda = \sqrt{m_N \hbar\omega}$, where m_N is the nucleon mass. For the two-body problem one defines a truncation of the model space that includes all the HO states with the quantum number $N = 2n + l \leq N_{max}$, where n (l) denotes the radial (angular-momentum) quantum number. Because we investigate here positive-parity states only, we limit N_{max} to even values. The usual definition of an ultraviolet cutoff Λ in the continuum can be extended to discrete HO states. Thus, in the HO basis, we define $\Lambda = \sqrt{m_N (N_{max} + 3/2)\hbar\omega}$ as the momentum associated with the energy of the highest HO level. A model space is defined by the two cutoffs. Within each model space we fix the parameters of the EFT to reproduce a set of observables and then calculate other observables in the same spaces. Because we construct the effective interaction directly in the model space, no additional unitary transformation is required, as it is in the conventional NCSM approach [2]. Contrary to the latter, here the effective interaction does not have to converge to an underlying "bare" interaction. What is important is the behavior of observables with the variation of the ultraviolet cutoff Λ. In each order in the power counting one expects independence of the physical observables with respect to Λ, within the theoretical errors induced by the absence of the higher-order operators that come at the next orders. There might also be a dependence on the infrared cutoff λ, which is an artifact of using a HO basis and should be removed. The infrared cutoff in this case is analogous to the inverse of the lattice size in a lattice discretization [17]. Obviously, as $\Lambda = \lambda\sqrt{N_{max} + 3/2}$, the running of the observables with Λ cannot be obtained by increasing $\hbar\omega$ arbitrarily in a fixed-N_{max} model space, as this procedure increases the infrared cutoff as well, introducing additional errors. Instead, we verify explicitly that cutoff dependences decrease with increasing Λ and decreasing λ, and we remove the influence of the infrared cutoff by extrapolating to the continuum limit, where $\hbar\omega \to 0$ with $N_{max} \to \infty$ so that Λ is fixed. Traditional shell-model calculations use larger values for the HO frequencies, of the order of $41/A^{1/3}$ MeV, but in our approach, we are interested in a small infrared cutoff limit, which removes the HO frequency dependence. At the end, we also extrapolate to the $\Lambda \to \infty$ limit.

Our method can be applied to either pionful or pionless EFTs. For simplicity, in this first application we limit ourselves to the pionless EFT in LO. The interaction in each model space has the same structure, *i.e.*, matrix elements of the contact two- and three-body interactions. The strengths of the three coupling constants have to be adjusted to reproduce three experimental observables, which here we choose to be the energy levels of the lightest nuclei: in the NN $^3S_1$ channel we use the ^{2}H binding energy to determine one coupling constant, while the other NN coupling constant (in the $^1S_0$ channel) and the strength of the contact 3N term (in the $S_{1/2}$ channel) are determined so that one simultaneously describes correctly the ^{3}H and ^{4}He binding energies.

The three- and four-body problems are solved using a relative-coordinate code developed following Ref. [18]. For four particles, the largest model space we can handle has $N_{max} = 16$. The calculations are much more involved for $A \geq 5$, because the relative-coordinate approach becomes inefficient due to the extremely difficult anti-symmetrization. To overcome this issue, we use a Slater-determinant (SD) basis constructed from HO single-particle states. The contact NN and 3N interactions in the S channels are exactly transformed to a proton-neutron SD basis [19], and the many-body diagonalization is performed with the shell-mode code REDSTICK [20]. For ^{6}Li, investigated in this paper, the largest model space that we can handle when including 3N forces has $N_{max} = 8$, or, equivalently, $6\hbar\omega$ excitations allowed above the lowest configuration. (Note that a complete $N\hbar\omega$ basis allows an exact separation of the spurious center-of-mass excitations, although the SD basis is not translationally invariant.)

With the deuteron, triton and alpha-particle ground-state energies used as input to determine the effective interaction, the only energy levels that we can predict for $0s$ nuclei are the excited states of ^{4}He, which have not previously been calculated in the pionless EFT. In Fig. 1, we show the results for the excited-state energy of the first spin-parity $J^\pi = 0^+$, isospin $T = 0$, shorthanded $(0^+; 0)$, state in ^{4}He, as a function of the cutoff momentum Λ.

As we are interested in the limit of large Λ and small λ, and very large N_{max} calculations are prohibitive even for few particles, we extrapolate the results obtained at smaller N_{max} by fitting our results to $E_0(\hbar\omega) + A(\hbar\omega)/\Lambda$, as shown by the continuous lines in Fig. 1. The choice of the $1/\Lambda$ dependence is motivated by the same type of LO running of the bound-state energy in the two-body sector in the continuum [9]. Although we cannot exclude the appearance of a softer dependence on Λ due to discrete-space and many-body effects, we obtain a good fit with this simple formula. (As a check, we found no significant change when we added a term $\log(a_0\Lambda)/\Lambda$ to the

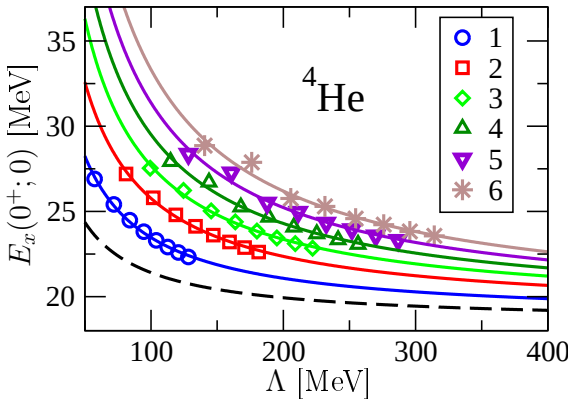

FIG. 1: (Color online) Dependence of the first $(0^+;0)$ excitation energy in ^{4}He on the ultraviolet momentum cutoff Λ. For each frequency $\hbar\omega$, given in the legend in MeV, we interpolate the direct results (discrete symbols) with a $1/\Lambda$ dependence (continuous curves). The dashed curve marks the limit $\hbar\omega \to 0$ (see text for details).

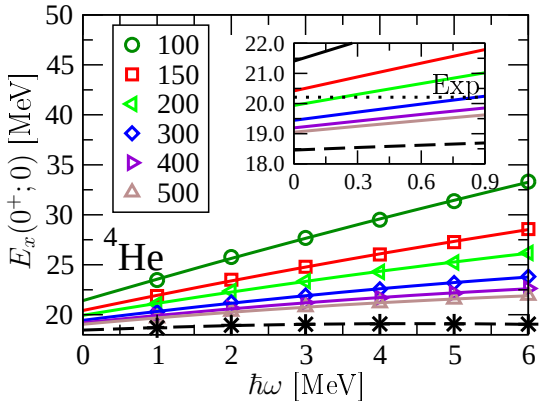

FIG. 2: (Color online) Dependence of the first $(0^+;0)$ excitation energy in ^{4}He on the infrared energy cutoff $\hbar\omega$. For each ultraviolet cutoff Λ, given in the legend in MeV, we interpolate as described in the text. The results marked with star symbols are obtained in the limit $\Lambda \to \infty$. In the insert we show the variation around origin, compared to the experimental value.

fit. More extensive calculations might be able to further pin down the running for the many-body system.)

We use the extrapolation above to study the λ dependence of the first $(0^+;0)$ energy. In Fig. 2, we present the results for selected ultraviolet-cutoff values, and also show the $\Lambda \to \infty$ limit, $E_0(\hbar\omega)$. Figure 2 shows a simple dependence upon the HO frequency. Thus, we interpolate the results for fixed Λ with second-degree polynomials. The coefficients of the squared dependence come out very small, so that the dependence is almost linear. The constant terms in the quadratic interpolation are then fitted ($\chi^2 \approx 10^{-4}$) with $E_0(0) + A(0)/\Lambda$. The resulting ultraviolet-cutoff dependence is shown as the dashed line in Fig. 1, and represents the continuum limit $\hbar\omega \to 0$. We find $E_0(0) = 18.5$ MeV, in remarkable (for a LO calculation) agreement with the experimental value 20.21 MeV [21]. We can perhaps understand this agreement if we consider that this state is very close to the four-nucleon continuum threshold, in an energy regime well within the validity of the pionless EFT.

Following the same procedure, the ground-state energy of ^{6}Li is evaluated, also for the first time in the pionless EFT. In this case, we obtain simultaneously several low-lying positive-parity states, irrespective of the spin or isospin values. Some $T = 0$ states appear degenerate in our calculation, which is not necessarily surprising, given that the spacing between levels is less than the expected error in the pionless EFT. However, we always obtain a single $(1^+;0)$ ground state, as found experimentally, its energy as function of Λ being given in Fig. 3. We remove the infrared-cutoff dependence using the same procedure as for ^{4}He. Although the fitting is subject to larger errors because of the limitation in N_{max}, and the quadratic dependence upon $\hbar\omega$ is more pronounced in the case of ^{6}Li, we obtain again a Λ^{-1} running in the continuum limit, as

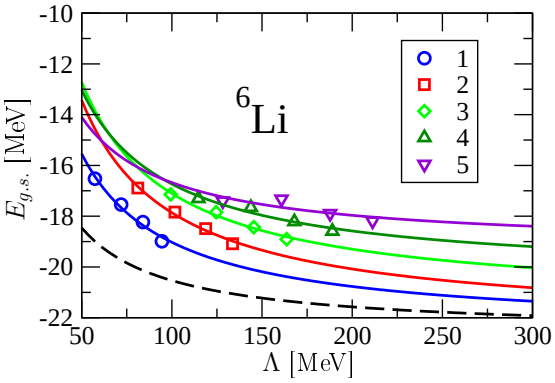

FIG. 3: (Color online) Same as in Fig. 1, but for the ground-state energy of ^{6}Li.

shown by the dashed curve in Fig. 3. For large values of the ultraviolet cutoff Λ, we estimate the binding energy as about 22.6 MeV, to be compared to the experimental result, 31.99 MeV [22]. While not as precise as the excited-state energy in ^{4}He, our result for the ^{6}Li binding energy is consistent with the expected LO errors in the pionless EFT.

We expect agreement to improve in higher orders, as in continuum calculations [7]. In LO, we were forced to use very large model spaces, restricting applicability to light systems. However, higher orders should produce reduced cutoff errors (that is, smaller coefficients of the $1/\Lambda$ term), faster convergence, and thus extended applicability to heavier systems. Since parameters multiply in subleading orders, a method to fit them to scattering data is desirable. However, because the basis states in the NCSM are constructed using HO wave functions, their bound-state asymptotics do not allow a direct determi-

nation of scattering observables. We are currently in the process of developing an approach to calculate scattering observables using a truncated HO basis [23].

Note that our results do not include Coulomb contributions explicitly. One-photon exchange between nucleons is non-perturbative only for momenta below about αm_N, where α is the fine-structure constant. Since nucleons in the bound states we consider have much larger typical momenta, electromagnetic interactions appear only in subleading orders. We thus used the observed ^{4}He binding energy as a fitting parameter; the difference between that and a Coulomb-corrected value is a higher-order effect. Of course, since they grow with the square of the number of protons, Coulomb effects are larger in heavier systems. In particular, we expect our ^{6}Li results to improve somewhat when we include Coulomb explicitly. This is because in our current calculation the Coulomb repulsion in ^{4}He is being divided through the number of nucleon pairs, and therefore implicit Coulomb effects are growing roughly as the square of the number of nucleons, rather than the number of protons as when Coulomb is included explicitly. A simple estimate suggests that this results in an underbinding of about 2 MeV in the ground-state energy of ^{6}Li. This 10% effect is, as expected, well in line with the size of subleading orders, but in itself would move the ^{6}Li energy to within 25% of the observed value.

In summary, we have investigated a new *ab initio* method for solving many-body problems in truncated model spaces. While our main application is to the description of properties of light nuclei, the principles are general, allowing similar treatment of other interacting quantum many-body systems. In our approach, the effective interaction is directly determined in the model space, where an exact diagonalization in a complete many-body basis is then performed. Power counting is seen as the justification for a cluster approximation. Our LO prediction for the energy of the first $(0^+;0)$ excited state in ^{4}He is within 10% of the experimental value, while the ^{6}Li ground-state energy is predicted at about 70% of the experimental value. These results are encouraging, and suggest that the method can be improved systematically by going to higher orders. The result in the six-nucleon system is considerably worse than for lighter systems, but is not in disagreement with the expected error in the pionless EFT at LO. Thus, more investigation is needed before any definitive conclusion can be drawn with regards to a possible breakdown of the pionless theory in heavier systems. In any case, applying the same procedure to the pionful EFT should increase the range of applicability of the method. Although we have not yet discussed other observables, the approach presented in this paper also offers the possibility of a consistent treatment of external operators on the same footing with the effective interaction, following the same general EFT principles.

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