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Novel Methods for Determining Effective Interactions for the Nuclear Shell Model

H. Mueller\textsuperscript{1}, J. Piekarewicz\textsuperscript{2}, and J.R. Shepard\textsuperscript{1}

\textsuperscript{1}Department of Physics, University of Colorado, Boulder, CO 80309
\textsuperscript{2}Department of Physics, Florida State University, Tallahassee, FL 32306
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Abstract

The Contractor Renormalization (CORE) method is applied in combination with modern effective-theory techniques to the nuclear many-body problem. A one-dimensional—yet “realistic”—nucleon-nucleon potential is introduced to test these novel ideas. It is found that the magnitude of “model-space” (CORE) corrections diminishes considerably when an effective potential that eliminates the hard-momentum components of the potential is first introduced. As a result, accurate predictions for the ground-state energy of the three-body system are made with relatively little computational effort when both techniques are used in a complementary fashion.

I. INTRODUCTION

The shell-model has long been the standard paradigm for treating the nuclear many-body problem. However, quite recently, the form of the shell model most frequently employed in practice has been criticized by Haxton and coworkers \cite{1,2}. The chief objection in these papers is that shell-model practitioners often use effective interactions which do not follow in any systematic way from realistic nucleon-nucleon (NN) interactions nor from the inevitable truncations that these entail. They point out that theoretical schemes exist that indicate how “bare” interactions should be modified to account for effects of truncations. Moreover, these schemes emphasize the necessity of using consistently modified operators rather than the bare ones used in many shell-model studies. Finally, they stress that tremendous recent advances in raw computational power and in numerical techniques now make it feasible to implement these theoretical schemes.

During the past few years, two of us (JP and JRS) have extensively studied low-dimensional quantum spin systems, especially the so-called spin-ladder materials \cite{3–7}. We note that interest in the study of the ladder compounds has been stimulated by suggestions that these deceptively simple materials could exhibit some of the critical behavior believed to be responsible for high-temperature superconductivity \cite{8}. In much of this work, we have made use of a novel “plaquette” basis and of a truncation scheme of the full Hilbert space that is suggested by the structure of this basis. Central to this work has been the use of the
COntactor REnormalization (CORE) method of Morningstar and Weinstein [9]. We have relied on CORE for the construction of an effective Hamiltonian and effective operators to be employed in concert with the truncated basis. Our success in applying CORE to important condensed-matter problems has inspired us to attempt adopting the approach to the nuclear-shell model as it directly addresses many of the concerns expressed in the preceding paragraph.

Another important development, the use of effective-field theories in nuclear physics, has been stimulated by novel ideas in modern renormalization theory [10,11]. Effective theories (ET’s) are low-energy approximations to the exact (and, thus, very complicated) theory. One of the central tenets behind ET’s is that a long-wavelength particle (of wavelength $\lambda$) should be insensitive to details of the potential at very short ($d \ll \lambda$) distances. Hence, it should be possible to replace the very complicated short-distance structure of the exact theory by a potential with a simpler short-range structure, while leaving the low-energy properties of the theory intact. The aim of this paper is to combine both approaches—CORE and effective theories—in a complimentary manner.

The paper has been organized as follows. In Sec. II we outline the basic steps in the implementation of CORE to the nuclear many-body problem. Particular emphasis is placed in the construction of the similarity transformation that generates the effective interaction. In the same section the basic ideas behind modern effective theories are introduced together with a detailed procedure on how to merge these two (CORE and ET’s) powerful approaches. In Sec. III we illustrate how the effective potential is constructed and the subsequent refinements of the basis that CORE entails. In particular, we focus on predictions of the ground-state energy of the three-body systems using a variety of approximations. Finally, our conclusions and plans for future calculations are presented in Sec. IV.

II. FORMALISM

In this section we describe in detail how CORE is to be used in the many-body problem. Central to the spirit of CORE is a similarity transformation that ultimately generates a renormalized Hamiltonian to be used in a severely truncated Hilbert space. We follow this discussion with a brief introduction to modern versions of effective theories placing particular emphasis on its use in combination with CORE.

A. CORE for the Shell Model

Here we will briefly outline the CORE method as adapted for the nuclear-shell model. The underlying dynamics is described by a non-relativistic Hamiltonian containing only two-body forces

$$H_A = \sum_{n=1}^{A} \frac{p_n^2}{2m} + \sum_{m<n}^{A} V(r_m-r_n), \quad (1)$$

where $V(r_m-r_n)$ is a realistic NN interaction. Because of potential problems with center-of-mass motion, the above Hamiltonian is modified by the introduction of a harmonic term that depends exclusively on the coordinate of the center of mass $\mathbf{R}$:
\[ V_\Omega^A(R) = \frac{1}{2} m A \Omega^2 R^2 . \] (2)

A many-body basis is then constructed from products of single particle harmonic oscillator wave functions characterized by the same oscillator frequency \( \Omega \). The modified \( A \)-body Hamiltonian, the standard starting point for most shell-model calculations [12], is now written as

\[
H_\Omega^A = \sum_{n=1}^{A} \left[ p_n^2 + \frac{1}{2} m \Omega^2 r_n^2 \right] + \sum_{m<n=1}^{A} \left[ V(r_m-r_n) - \frac{m \Omega^2}{2A} (r_m-r_n)^2 \right].
\] (3)

The terms depending on \( \Omega \) allow separation of the center-of-mass motion and, after trivial subtractions of the center-of-mass energy, the calculations yield the desired physical spectrum which ultimately is independent of \( \Omega \).

The first step in the implementation of CORE is the identification of an “elementary” block and a truncation scheme [9]. In our case the elementary block, or one-body term, consists of the single-nucleon Hamiltonian appearing in Eq. (3). This one-body term, henceforth denoted by \( h_1 \), defines the basis via products of one-body harmonic-oscillator eigenstates. Subsequently, the truncation scheme is defined by retaining only those states with energy less than some maximum (cutoff) value \( E_{\text{max}} \), or equivalently oscillator quanta less than some maximum value \( N \). In this way it is guaranteed, by construction, that the spectrum of the effective Hamiltonian \( h_1 \) reproduces identically the low-energy properties of the exact one-body Hamiltonian.

The next step involves computation of the effective Hamiltonian for the two-body system. To begin, the two-body problem must be solved exactly. This is accomplished by using a very large basis, \( i.e. \), a basis as large as can be afforded computationally and one characterized by a cutoff \( N_\infty \) which is effectively infinite. For the method to have any utility we evidently require \( N_\infty \gg N \). CORE now instructs us that the effective two-body Hamiltonian be given in terms of a similarity transformation:

\[
H_{\text{eff}}^{(1,2)} \equiv S E_{\text{diag}} S^T.
\] (4)

where \( E_{\text{diag}} \) is the diagonal matrix containing the lowest \( N \) exact eigenvalues of the two-body system where \( N \) is the number of two-body states defined by the cutoff \( N \). Evidently, the structure of \( H_{\text{eff}}^{(1,2)} \) guarantees, independent of the details of the similarity transformation, the low-energy spectrum of the full theory will be preserved. We now discuss the particular form of \( S \) prescribed by CORE.

By elementary linear algebra, the columns of the similarity transformation are the eigenvectors of \( H_{\text{eff}}^{(1,2)} \). CORE demands that the first column of \( H_{\text{eff}}^{(1,2)} \), \( i.e. \), the eigenvector associated with the lowest eigenvalue, has a non-zero overlap with the lowest \( \text{exact} \) eigenvector of the full Hamiltonian. A simple way to implement this demand is by choosing the first eigenvector in the model space to be proportional to the lowest exact eigenvector after it has been truncated and then properly normalized. To construct the second column of the similarity transformation one starts with the second exact eigenvector, truncates it and then, via a Gram-Schmidt procedure, subtracts any component parallel to the first column. This procedure guarantees the fulfillment of another important CORE requirement: the \( n^{\text{th}} \) eigenvector in the model space must have a non-zero overlap with the \( n^{\text{th}} \)-lowest exact
eigenvector yet no such overlap is allowed with the previous \( n - 1 \) eigenstates. The third column is determined in a similar way and must have no component parallel to the first two. This process is repeated until the \( N \) columns of \( S \) are completely determined. Note that, in practice, Gram-Schmidt is numerically unstable and more sophisticated—but, in principle, equivalent—techniques must be used \[9\]. Finally the effective two-body interaction is obtained by subtracting the one-body terms from \( H_{\text{eff}}(1, 2) \):

\[
V_{\text{eff}}(1, 2) = H_{\text{eff}}(1, 2) - h_1(1) - h_1(2) .
\] (5)

Hence, the effective 2-body Hamiltonian to be used in the truncated model space is given by

\[
H_{\text{eff}}^{(2)} = \sum_{n=1}^{A} h_n + \sum_{m<n=1}^{A} V_{\text{eff}}(m, n) .
\] (6)

It is possible to construct three-body, four-body, etc, interactions by similar methods. Indeed, this is essential if many-body properties are to be reproduced exactly. Note that the induced many-body interactions appear as a consequence of truncations even when the original nuclear Hamiltonian contains at most two-body terms as in Eq. (1). The usefulness of the approach depends, of course, on being able to stop at a low order in the cluster expansion while retaining acceptable accuracy.

**B. CORE and Effective Theories**

Effective Theories (ET’s) are now widely employed in many fields of physics including nuclear theory \[11\]. The philosophical similarities between CORE and ET’s are obvious: in both cases one attempts to incorporate in a systematic fashion the contributions from short-ranged (high momentum/energy) physics into effective interactions and operators that are defined in a Hilbert space which excludes the high momentum/energy states. Indeed, Bogner and Kuo \[13\] have recently examined the connection between CORE-like approaches, such as Lee-Suzuki \[14–16\] and Krenciglowa-Kuo \[17\] schemes on one hand and ET’s on the other. We are presently undertaking similar studies using concepts from CORE and renormalization-group (RG) methods outlined by Birse and collaborators \[18\]. Our results will appear in a future publication.

In the present work we examine how CORE and the methods of ET can be applied to the shell-model problem in a *complementary* manner. The basic idea is as follows: the bare \( NN \) interaction (see, e.g., Ref. \[19\]) is pathological in the sense that it is characterized by a very strong short-range repulsion. Obtaining accurate many-body energies using the bare interaction therefore requires huge bases. CORE and other similar methods are used to remedy this problem. We propose to solve this problem by first constructing an effective \( NN \) potential of a convenient form for use in shell-model calculations. The main theoretical underpinning behind effective theories is that a long-wavelength particle should be insensitive to details of the short-range interaction. Thus, one adds new (smoother) interactions to “mimic” the effects of the unknown short-distance physics. Since no explicit short-range contributions will appear in the effective potentials, one expects smaller bases to be sufficient. Moreover, there is no reason that CORE cannot be used together with an effective
potential to further refine the basis, a strategy that may result in substantially increased computational efficiency.

Our determination of the effective potential follows from the procedures outlined by Lepage \[10\] and those later adapted by Steele and Furnstahl \[20,21\] to treat the \(NN\) interaction. For simplicity we work in one dimension and treat all particles as spinless and distinguishable; they are assumed to have identical masses of \(m = 939\) MeV. We assume a bare \(NN\) interaction with the same pathologies of a realistic interaction. That is, it is given by the sum of a strong short-range repulsive exponential and a medium-range attractive exponential:

\[
V(x) = V_s e^{-m_s|x|} + V_v e^{-m_v|x|}.
\]

(7)

The two masses were chosen to be equal to \(m_s = 400\) MeV and \(m_v = 783\) MeV, respectively. The strengths of the potentials, \(V_s = -506\) MeV and \(V_v = +1142.49\) MeV, were chosen to give a binding energy and point root-mean-square (rms) radius for the symmetric (“deuteron”) state of \(E_b = -2.2245\) MeV and \(r_{\text{rms}} = 1.875\) fm and \(\sqrt{\left\langle r^2 \right\rangle} = 1.875\) fm, respectively. Note that for the \(NN\) system an odd-parity state bound by \(-0.180358\) MeV is also found and that the three body ground state for this potential is bound by \(-6.32\) MeV.

Employing an option suggested by Lepage \[10\], we choose a gaussian form for our effective potential:

\[
V_{\text{eff}}(x) = \frac{1}{a} \left( c + d \frac{\partial^2}{\partial \xi^2} + e \frac{\partial^4}{\partial \xi^4} + \ldots \right) \exp(-\xi^2) ; \quad \xi \equiv x/a.
\]

(8)

The range parameter has been fixed at \(a = 1.16\) fm as it reproduces the deuteron binding energy exactly. Yet, as indicated in Fig. 1, variations of this quantity—with the corresponding adjustment of the effective parameters to reproduce the low-energy phase shifts—have very little effect on the deuteron binding energy and, indeed, on any of our calculations of low-energy properties. Note that the parameters of the effective potential \((c, d,\) and \(e)\) are fixed separately for the even and odd channels. They are constrained to reproduce the low-energy scattering phase shifts for the appropriate channel, as we explained below.

III. RESULTS

Following the discussions in Ref. \[20,21\], we fit the parameters of \(V_{\text{eff}}\) to quantities which yield the effective range expansion when expanded in even powers of the wavenumber, \(k\). In one dimension we find for the even channel

\[
k \tan \delta_e(k) = + \frac{1}{a_e} + \frac{r_e}{2} k^2 + \mathcal{O}(k^4).
\]

(9)

where \(\delta_e\) is the even-channel phase shift and \(a_e\) and \(r_e\) are the scattering-length and effective-range parameters, respectively. This apparently unorthodox form of the effective-range expansion emerges from the fact that, in one dimension, the symmetric wave-function does not vanish at the origin. For the odd channel we find the familiar expression

\[
k \cot \delta_o(k) = - \frac{1}{a_o} + \frac{r_o}{2} k^2 + \mathcal{O}(k^4).
\]

(10)
We have found that including only the first two terms of Eq. (8) for $V_{\text{eff}}$ gives, as expected, an excellent reproduction of both scattering-lengths and effective-range parameters. The parameters of the effective potential are shown in Table || along with the binding energies obtained using the bare and effective potentials. The resulting $V_{\text{eff}}$'s for various orders of Eq. (8) are compared with the bare potential in Fig. 2. Insofar as the low-energy properties of the theory are concerned, the smooth $V_{\text{eff}}$ is practically indistinguishable from the exact, and very pathological, $V_{\text{bare}}$. As Table || indicates, the effective potentials reproduce the exact binding energies very accurately. That the effective potentials do so without possessing the "pathologies" of the bare $NN$ potential alluded to earlier is demonstrated in Fig. 3. The exact binding energy for the even-parity state is determined accurately by solving the Schrödinger equation using the Numerov algorithm. This energy is also determined by evaluating the matrix elements of the potential in a harmonic-oscillator basis and then diagonalizing the matrix. Fig. 3 shows that, as suggested above, such calculations using $V_{\text{eff}}$ converge much faster than with the bare interaction where, eventually, round-off errors cause discrepancies to grow as the basis size increases.

Finally, we turn to the three-body system which represents the testing ground for our model. Using the bare potential with very large basis sizes ($N \simeq 100$) and then extrapolating to $N \to \infty$, we find an exact ground-state energy for the three-body system of $-6.32$ MeV. Table || summarizes approximate calculations of this quantity employing severely truncated bases; i.e., $N \leq 30$. (Note that the number of three-body states scales roughly like $N^3$.) The same information also appears in Fig. 4. Four types of calculations are reported: calculations using either the bare or effective $NN$ interaction both with and without CORE. The results show clearly that CORE corrections are important, especially for small values of $N_{\text{basis}}$. Yet these corrections are significantly more important for the bare potential than for the effective one. This is to be expected as, in constructing the effective interaction, we have already "softened" the potential to such a degree that most of its large momentum components are absent. Put another way, the smoothed effective potential does not explicitly contain the "pathological" short-range contributions which CORE must treat. At the same time, the convergence to the exact ground-state energy is much faster overall for the effective interaction. Note that this is true even when one considers that the exact binding energy of the three-body system for the effective potential ($-6.89$ MeV) differs slightly from the exact three-body energy for the bare interaction ($-6.32$ MeV). Presumably, this difference is due to the omission of induced three-body interactions. This relatively small discrepancy suggests that such three-body interactions are tractably small.

IV. CONCLUSIONS

A contractor renormalization (CORE) approach has been applied in concert with modern versions of effective theories (ET’s) to the nuclear many-body problem. CORE is a "model-space" approach similar to existing techniques, such as the Lee-Suzuki method, that have been applied already with some success to the nuclear many-body problem. The central concept behind CORE is a similarity transformation responsible for generating a renormalized Hamiltonian with identical low-energy properties to the exact Hamiltonian. The initial study presented here has been limited, for simplicity, to one spatial dimension. Yet the bare nucleon-nucleon potential employed throughout the paper possesses the same
“pathologies”—the short-range repulsive core—as any realistic interaction. To remove these pathologies we proceeded as follows. First, the high-momentum components of the potential were removed through the introduction of an effective potential that was constrained—in effect—by low-energy scattering phase shifts. Such an effective potential predicts a two-body (“deuteron”) bound-state energy identical to that obtained with the bare interaction. Second, in calculating the ground-state energy of the three-body system we depended on CORE to compensate for severely truncating the size of the basis employed in the calculation. In computing the ground-state energy of the three-body system we observed that, as in most implementations of model-space techniques, CORE corrections improve significantly the convergence towards the exact ground-state energy. However, use of the effective two-body potential significantly accelerated the rate of convergence while simultaneously reducing the magnitude of the CORE corrections.

Overall these results are gratifying as they suggest that ET’s can be profitably combined with more traditional model-space methods for use with the nuclear shell model. For us, much remains to be done. Apart from the obvious extension to more realistic systems, we must determine how to optimally mesh ET and CORE as well as how to correct operators in a manner consistent with the construction of the effective potential. Also, a preliminary comparison between CORE and a commonly used [12] approach for evaluating effective interactions—the Lee-Suzuki method—has been made by us. We find that, at least for the one-dimensional three-body system treated here, the two methods give similar results, with ground-state energies computed using CORE being slightly—but consistently—closer to the exact value. (See Fig. 5 for relevant comparison with relatively small basis sizes.) In a future study we intend to elucidate the relationships between CORE, Lee-Suzuki, and other related approaches such as the Krenciglowa-Kuo scheme [17]. The formalism developed by Andreozzi [23] may prove useful in this regard. Finally, as mentioned earlier, it would be very useful and informative to find a set of RG-like equations [18] which would lead directly to a sufficiently accurate version of $V_{\text{eff}}$. Illuminating early steps in this direction may be found in Refs. [2,13,24–26].

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FIG. 1. The flow of the parameters of $V_{\text{eff}}$ as a function of the cutoff $\Lambda = 1/a$. Also shown is the evolution of the two-body (deuteron) binding energy. The value of $a = 1.16$ fm (or $\Lambda = 170$ MeV) was chosen for all remaining calculations as it reproduces the deuteron binding energy exactly.
FIG. 2. The one-dimensional potentials used in our two- and three-body calculations. The bare potential yields a “deuteron” with the correct binding energy and point radius which qualitatively resembles the $^1S_0$ av18-potential \([19]\). Also shown are the lowest (only $c \neq 0$ in Eqn. \([8]\)), next-to-lowest (only $c$ and $d \neq 0$) and next-to-next-to-lowest order (only $c$, $d$ and $e \neq 0$) fits for the even channel.
FIG. 3. Differences between the exact binding energy of the one-dimensional deuteron as determined by direct solution of the Schrödinger equation and the energies determined by diagonalization in harmonic-oscillator bases of various sizes are displayed. Results using the bare and effective potentials are compared and reveal superior convergence using the latter.
FIG. 4. Ground-state energies for the three-body system in one spatial dimension using the bare and effective interactions with basis size determined by $N_{\text{basis}}$. Results are shown with and without using CORE. The exact three-body ground-state energy is $-6.32$ MeV.
FIG. 5. Ground state energies for the 1D three-body system using relatively small basis sizes determined by $N_{\text{trunc}}$. Results using the uncorrected bare potential are compared with those obtained using interactions corrected for truncations by two different model-space methods, namely CORE \cite{9} and the more commonly used Lee-Suzuki method \cite{15,16}. All energies are in MeV; the exact three body ground state energy is -6.32 MeV.
TABLES

| Channel | $c$   | $d$   | BE (bare)   | BE (eff)   |
|---------|-------|-------|-------------|------------|
| Even    | -0.039342 | -0.159944 | -2.2245 MeV | -2.2245 MeV |
| Odd     | -0.301863  | -0.104362  | -0.1802 MeV  | -0.1802 MeV  |

TABLE I. Parameters of $V_{\text{eff}}$ [see Eq. (8)] for even and odd channels. Also shown are the binding energies using the bare and effective $NN$ interactions for a gaussian-cutoff value of $a=1.16$ fm.

| $N_{\text{basis}}$ | Bare–no CORE | Bare–with CORE | Effective–no CORE | Effective–with CORE |
|---------------------|--------------|---------------|-------------------|---------------------|
| 10                  | +6.2568      | +0.9258       | -1.0741           | -1.9028             |
| 20                  | -3.9889      | -4.5934       | -5.5396           | -5.6624             |
| 30                  | -5.4477      | -5.6327       | -6.4284           | -6.4606             |

TABLE II. Ground-state energies for the one-dimensional three-body system using the bare and effective interactions with basis size determined by $N_{\text{basis}}$. Results are shown with and without using CORE. When CORE was used, the size of the original basis was $N_{\infty}=50$. All energies are in MeV, with the exact three-body ground-state energy being $-6.32$ MeV.