Morphing the Shell Model into an Effective Theory

W. C. Haxton and C.-L. Song

Institute for Nuclear Theory, Box 351550, and Department of Physics, University of Washington, Seattle, Washington 98195

(Received 26 July 1999)

We describe a strategy for attacking the canonical nuclear structure problem—bound-state properties of a system of point nucleons interacting via a two-body potential—which involves an expansion in the number of particles scattering at high momenta, but is otherwise exact. The required self-consistent solutions of the Bloch-Horowitz equation for effective interactions and operators are obtained by an efficient Green's function method based on the Lanczos algorithm. We carry out this program for the simplest nuclei, d and ^{3}He, in order to explore the consequences of reformulating the shell model as a controlled effective theory.

PACS numbers: 21.60.–n, 11.10.Ef, 24.10.Cn, 27.10.+h

In this Letter we argue that it may be possible to move beyond the nuclear shell model (SM) to a more rigorous treatment of the canonical nuclear structure problem of A nonrelativistic point nucleons interacting via a two-body potential. Our optimism is inspired by several recent developments. One is the success of the Argonne group's efforts [1] to predict the properties of light nuclei in effectively exact Green's function Monte Carlo (GFMC) calculations, using an NN potential carefully fit to scattering data and augmented by weaker three-body forces. This suggests that SM failures have their origin in an incomplete treatment of the many-body physics, rather than in the starting Hamiltonian. A second is the success of effective field theory (EFT) treatments [2] of the two- and three-body problems. This work not only provides some insight into why such a starting Hamiltonian is reasonable, but has made the community more aware of the uncontrolled approximations implicit in the SM and other approaches.

The SM's strength is its explicit representation of $\sim$60% of the wave function that resides at long wavelengths: the A-body correlations important to collective modes are addressed by direct diagonalization. A third development is the remarkable recent advances in such SM technology, including Lanczos-based methods [3], treatments of light nuclei involving many shells [4], and Monte Carlo sampling algorithms [5,6]. The dimensions of tractable SM spaces have risen by several orders of magnitude in the past few years.

Such diagonalizations in a long-wavelength "included space" could be an important piece of a rigorous effective theory (ET) of nuclear structure in which the Hamiltonian operating in an infinite Hilbert space

$$H = \frac{1}{2}\sum_{i,j=1}^{A}(T_{ij} + V_{ij}) \rightarrow \frac{1}{2}\sum_{i,j,\ldots=1}^{A} H^{\rm eff}_{ij\ldots} \qquad (1)$$

is replaced by an $H^{\rm eff}$ operating in a finite SM space. The effects of high momentum components appear as effective contributions to the Hamiltonian and operators. The hope in nuclear physics, inspired by Brueckner's treatment of nuclear matter, is that the "excluded space" integration might be carried out as a rapidly converging series in the number of nucleons scattering at one time in high momentum states. In this way the effective theory might prove far more tractable than the original A-body problem in an infinite Hilbert space.

The SM is a very successful model, but not a controlled ET: SM effective interactions are most commonly determined phenomenologically and thus containing adjustable parameters not connected with the underlying Hamiltonian [7]. However, we will argue that it is possible to morph the SM into a faithful ET while preserving the elegant technology of the original model. The result is an ET with very attractive properties, while the cost is a manageable degree of additional complexity:

(1) The functional form of the SM effective interaction, $\langle\alpha\beta|H^{\rm eff}|\gamma\delta\rangle$, is appropriate in an ET only in lowest order and only if the calculation is restricted to a single shell [7]. In a faithful ET three-, four-, and higher-body operators are successively added, and the matrix elements generally carry, in addition to single-particle quantum numbers, an index specifying the number of quanta carried by the remaining spectator nucleons.

(2) SM wave functions are orthogonal and normed to unity. In ET the effective wave functions are naturally defined as the restrictions of the true wave functions $|\Psi_i\rangle$ to the model space. The norms are calculable and less than unity, and orthogonality is lost.

(3) Because SM $H^{\rm eff}$s are usually derived phenomenologically, there is no diagrammatic basis for generating the effective operator. Thus empirical operator renormalizations must also be introduced, limiting the model's predictive power. In an ET effective operators are calculated diagrammatically, and are consistent with $H^{\rm eff}$.

In this Letter we describe the first steps in an effort to assess the feasibility of an exact ET "SM"-like theory. The approach is sketched in Fig. 1. The Hilbert space is divided into a long-wavelength SM space, defined by some energy scale $\Lambda_{\rm SM}$, and a high-momentum space. One can

 0031-9007/00/84(24)/5484(4)$15.00

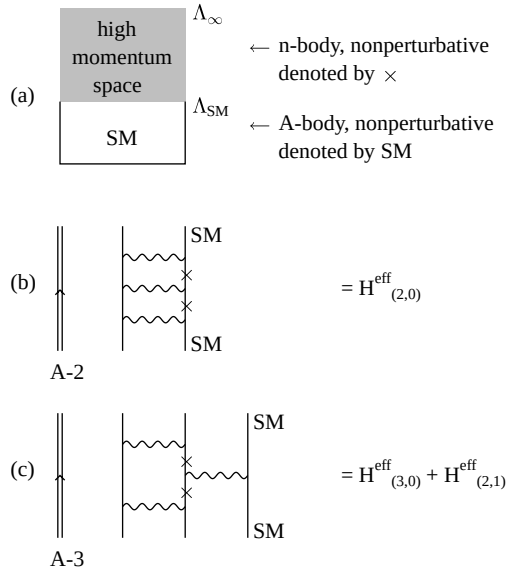

FIG. 1. Cluster expansion of the effective interaction.

truncate the latter at some scale $\Lambda_\infty \sim 3$ GeV, characteristic of the cores of realistic potentials, as above this energy, excitations make a negligible contribution. All correlations within the SM space are included, but the high-momentum correlations in the excluded space are limited to n body, where n is the cluster size. Thus Figs. 1b and 1c give the lowest and next-to-lowest approximations to $H^{\rm eff}$. Note that one can view Fig. 1c as containing Fig. 1b, a density-dependent two-body correction to Fig. 1b, and true three-body terms. The pattern continues as n is increased: true n-body terms are introduced and all lower-order results are corrected to one higher order in the density ρ.

The diagram in Fig. 1b is almost the usual two-body effective interaction: the difference is that the noninteracting A-2 nucleons do influence whether the A nucleons reside below $\Lambda_{\rm SM}$, leading to a multivalued $H^{\rm eff}$. This point is discussed in some detail in [7]. Figure 1c is the generalization to a three-body cluster, and implies that some technique is available to sum this three-body ladder nonperturbatively.

If the SM space is defined as all harmonic oscillator Slater determinants with $E \le \Lambda_{\rm SM}$, $H^{\rm eff}$ becomes translationally invariant and the ladder sums can be carried out in relative coordinates, a considerable simplification. The projection operator onto the high-momentum space Q thus depends on $\Lambda_{\rm SM}$ and the oscillator parameter b, where the latter can be chosen to optimize the convergence in Λ_∞ [8].

The resulting Bloch-Horowitz (BH) equation [9] is then

$$H^{\rm eff} = H + H\,\frac{1}{E - QH}\,QH\,, \qquad H^{\rm eff}|\Psi_{\rm SM}\rangle = E|\Psi_{\rm SM}\rangle, \quad |\Psi_{\rm SM}\rangle = (1 - Q)\,|\Psi\rangle\,, \tag{2}$$

where $|\Psi\rangle$ is the exact wave function and $H|\Psi\rangle = E|\Psi\rangle$. These equations must be solved self-consistently because $H^{\rm eff}$ depends on the unknown eigenvalue E. The harmonic oscillator appears only implicitly through Q in distinguishing the long-wavelength SM space from the remainder of the Hilbert space.

There is extensive literature on this and similar equations [10,11]. Frequently H is divided into an unperturbed H_0 and a perturbation $H - H_0$, but well-known pathologies due to intruder states can affect the resulting perturbation expansion [12]. The approach explored here is nonperturbative and uses the Lanczos algorithm to sum the n-body ladders.

The Lanczos algorithm recursively maps a Hermitian operator H of dimension N into tridiagonal form

$$\begin{aligned} H|v_1\rangle &= \alpha_1|v_1\rangle + \beta_1|v_2\rangle\,, \\ H|v_2\rangle &= \beta_1|v_1\rangle + \alpha_2|v_2\rangle + \beta_2|v_3\rangle\,, \\ H|v_3\rangle &= \beta_2|v_2\rangle + \alpha_3|v_3\rangle + \beta_3|v_4\rangle, \ldots\,. \end{aligned} \tag{3}$$

If this process is truncated after $n \ll N$ steps, the resulting matrix contains the information needed to reconstruct the exact $2n - 1$ lowest moments of $|v_1\rangle$ over the eigenspectrum. One of the applications of this algorithm is in constructing fully interacting Green's functions [13] as a function of E,

$$\frac{1}{E - H}\,|v_1\rangle = g_1(E)\,|v_1\rangle + g_2(E)\,|v_2\rangle + \cdots\,, \tag{4}$$

where the $g_i(E)$ are continued fractions that depend on α_i, β_i and where E appears only as a parameter.

Thus a simple procedure can be followed to solve the BH equation:

(i) For each relative-coordinate vector in the SM space $|\gamma\rangle$, form the excluded-space vector $|v_1\rangle \equiv QH|\gamma\rangle$ and the corresponding Lanczos matrix for the operator QH. Retaining the resulting coefficients α_i, β_i for later use, construct the Green's function for some initial guess for E and then the dot product with $\langle\gamma'|H$ to find $\langle\gamma'|H^{\rm eff}(E)\,|\gamma\rangle$.

(ii) Perform the SM calculation to find the desired eigenvalue E' which, in general, will be different from the guess E. Using the stored α_i, β_i, recalculate the Green's function for E' and $H^{\rm eff}(E')$ then redo the SM calculation. The process is repeated until the energy is fully converged.

(iii) Then proceed to the next desired bound state and repeat the process. Note that it is not necessary to repeat the $H^{\rm eff}$ calculation. The eigenvalue taken from the SM calculation is, of course, that of the next desired state, yielding a distinct $H^{\rm eff}$ for each eigenvalue.

The attractiveness of this approach is that the effective interaction part of the procedure, which is relatively time consuming as it requires one to perform a large-basis Lanczos calculation for each relative-coordinate starting vector in the SM space, is performed only once. $H^{\rm eff}$ is then known as a function of E, allowing one to iterate to self-consistency without further Lanczos work, and to treat a series of bound states. To achieve self-consistency the SM step must be repeated in the iterations, but this

TABLE I. ET results for the ^{3}He ground state wave function calculated with the Argonne $v18$ potential. Selected basis states are designated somewhat schematically as $|N, \alpha\rangle$, where N is the total number of oscillator quanta and α is an index representing all other quantum numbers.

State	Amplitude					
	$0\hbar\omega$ (31.1%)	$2\hbar\omega$ (57.4%)	$4\hbar\omega$ (70.0%)	$6\hbar\omega$ (79.8%)	$8\hbar\omega$ (85.5%)	Exact (100%)
$\|0,1\rangle$	0.55791	0.55791	0.55791	0.55795	0.55791	0.55793
$\|2,1\rangle$	0.00000	0.04631	0.04613	0.04618	0.04622	0.04631
$\|2,2\rangle$	0.00000	−0.48255	−0.48237	−0.48243	−0.48243	−0.48257
$\|2,3\rangle$	0.00000	0.00729	0.00731	0.00730	0.00729	0.00729
$\|4,1\rangle$	0.00000	0.00000	−0.02040	−0.02042	−0.02043	−0.02047
$\|4,2\rangle$	0.00000	0.00000	0.11267	0.11274	0.11275	0.11289
$\|4,3\rangle$	0.00000	0.00000	−0.04191	−0.04199	−0.04208	−0.04228

step is not time consuming and the convergence is rapid (6–8 cycles, typically). For example, modern work stations can manage SM calculations of dimension 10^6 in about 30 min.

The technical aspects of this approach are described elsewhere [8,14]. Here we focus on the results for the simplest nuclei, d and ^{3}H, carrying the above process to completion (two- and three-body ladders, respectively).

The binding energies and operator matrix elements for simple systems like ^{3}He can, of course, be calculated exactly by other methods. The point of our work is not to offer an alternative to these techniques for these nuclei, but rather to illustrate the conceptual differences between a faithful ET and the SM. We performed d and ^{3}He ET calculations for a series of SM spaces ($2\hbar\omega$, $4\hbar\omega$, $6\hbar\omega$, and $8\hbar\omega$), in each case using the Lanczos Green's function algorithm to evaluate the two- and three-body ladders (100 Lanczos iterations are more than sufficient) and iterating the SM calculation until the results are fully converged. The deuteron calculation is rather trivial; for $\Lambda_\infty \sim 60\hbar\omega$ the ^{3}He calculation involves a dense matrix of dimension $\sim 2 \times 10^4$, still quite modest by current SM standards. (The Hamiltonian matrix is dense because relative Jacobi coordinates are used, rather than the m scheme, together with standard Talmi-Brody-Moshinsky methods [14,15].)

A correct ET should give results that are independent of how one chooses to divide the Hilbert space, e.g., the choices of $\Lambda_{\rm SM}$ and b. The dependence on b is explored in [8]. In the case of $\Lambda_{\rm SM}$, the deuteron binding energies for the four chosen SM spaces agreed to four places, -2.224 MeV (using $\sqrt{2}\,b = 1.6f$ and $\Lambda_\infty = 140\hbar\omega$). The exact result is -2.2246 MeV. The ^{3}He binding energy (for $\Lambda_\infty = 60\hbar\omega$) is -6.871 MeV, which compares with the GFMC result of -6.87 ± 0.03 MeV. Because the effective interactions calculation is otherwise exact, the results are variational in Λ_∞, approaching the exact answer from above. The dependence is very smooth, varying as $\exp(-a\Lambda_\infty^2)$ [8]. This allows us to predict a ^{3}He binding energy for asymptotic Λ_∞ of -6.906 MeV.

A more interesting test is the evolution of the wave function as the SM space is enlarged. Table I gives results for ^{3}He. (The procedure for calculating the wave function normalization is discussed below.) Unlike typical SM calculations, the amplitudes agree over overlapping pieces of the Hilbert spaces. As one proceeds through $2\hbar\omega, 4\hbar\omega, 6\hbar\omega, \ldots$ calculations, the ET wave function evolves only by adding new components in the expanded space. Consequently, as Table I shows, the wave function norm grows.

This evolution will not arise in the standard SM because the wave function normalization is set to unity regardless of the model space. It will also not arise for a second reason, illustrated in Table II. The three-body ^{3}He matrix elements of $H^{\rm eff}$ are crucially dependent on the model space: a typical matrix $\langle\alpha|H^{\rm eff}|\beta\rangle$ changes very rapidly under modest expansions of the model space, e.g., from $2\hbar\omega$ to $4\hbar\omega$. Yet it is common practice in the SM to expand calculations by simply adding to an existing SM Hamiltonian new interactions that will mix in additional shells. We suspect the behavior found for ^{3}He is generic in ET calculations: it arises because a substantial fraction of the wave function lies near but outside the model space (e.g., see Table I). An expansion of the model space changes the energy denominators for coupling to some of these configurations, and moves other nearby configurations from the excluded space to the model space. Naively, relative changes in effective interaction matrix elements of unity are expected.

Now we turn to the question of operators. The standard procedure in the SM is to calculate nuclear form factors with bare operators, or perhaps with bare operators renormalized according to effective charges determined phenomenologically at $q^2 = 0$, using SM wave functions normed to 1. As we now have a series of exact effective

TABLE II. Selected BH three-body effective interaction matrix elements for ^{3}He, in MeV, illustrating the strong dependence on the SM space.

	$2\hbar\omega$	$4\hbar\omega$	$6\hbar\omega$	$8\hbar\omega$
$\langle 0,1\|H^{\rm eff}\|2,1\rangle$	−4.874	−3.165	−0.449	1.279
$\langle 0,1\|H^{\rm eff}\|2,5\rangle$	−0.897	−1.590	−1.893	−2.208
$\langle 2,1\|H^{\rm eff}\|2,2\rangle$	6.548	−2.534	−4.144	−5.060

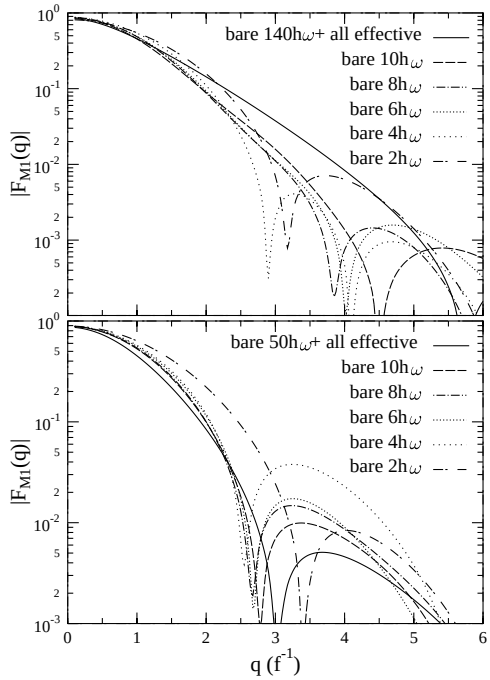

FIG. 2. The magnetic elastic form factors for the deuteron (top) and ^{3}He (bottom) calculated with the exact H^{eff}, SM wave functions normalized to unity, and a bare operator are compared to the exact result (solid line). When effective operators and the proper wave function normalizations are used, all results become identical to the solid line.

interactions corresponding to different model spaces, we can test the validity of this approach. The results for the elastic magnetic form factors are given in Fig. 2. Even though each SM H^{eff} is, in a sense, perfect, the results for bare operators are widely divergent at even modest momentum transfers of $\sim 2/f$. This is not surprising: if an operator transfers a momentum $q \gtrsim 2k_F$ to the nucleus, where k_F is the Fermi momentum, the resulting amplitude should reside primarily outside the SM space, where it contributes only through effective pieces of the operator.

Clearly the effective interaction and effective operator have to be treated consistently and on the same footing. The bare operator $\hat{O}$ must be replaced by

$$\hat{O}^{\text{eff}} = \left(1 + HQ\,\frac{1}{E_f - HQ}\right)\hat{O}\left(1 + \frac{1}{E_i - QH}\,QH\right) \tag{5}$$

and must be evaluated between SM wave functions normed according to

$$1 = \langle \Psi_i \,|\, \Psi_i \rangle = \langle \Psi_i^{\text{SM}} | \hat{1}^{\text{eff}} | \Psi_i^{\text{SM}} \rangle \tag{6}$$

(and similarly for $|\Psi_f^{\text{SM}}\rangle$). These expressions can be evaluated with the Lanczos Green's function methods described earlier. When this is done, all of the effective calculations, regardless of the choice of the model space, yield the same result, given by the solid lines in Fig. 2.

It seems likely to us that many persistent problems in nuclear physics—such as the renormalization of g_A in β decay—could be associated with the failure of the SM to deal with the questions of wave function normalization and effective operators. If so, then such issues will not be resolved unless we can morph the SM into a more controlled theory where effective interactions and operators can be addressed consistently.

In conclusion we point out that the ability to solve the three-body problem as an exact ET in a SM-like model space is already a significant step towards treating heavier nuclei: it implies an ability to handle effective interactions and operators correctly at the level of three-body clusters. An attempt will be made to extend the current work to $A = 4$ and then to imbed the results in such a SM-like cluster expansion. Whether and how well such a Brueckner expansion will converge are open questions.

This work was supported in part by the Division of Nuclear Physics, U.S. Department of Energy. We thank David Kaplan, Peter Lepage, and Martin Savage for helpful comments.

[1] R. B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995); B. S. Pudliner *et al.*, Phys. Rev. C **56**, 1720 (1997).
[2] D. B. Kaplan, M. Savage, and M. Wise, Nucl. Phys. **B534**, 329 (1998).
[3] E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, J. Retamosa, and A. P. Zuker, Phys. Rev. C **59**, 2033 (1999), and references therein.
[4] P. Navratil and B. R. Barrett, Phys. Rev. C **57**, 562 (1998); **59**, 1906 (1999).
[5] S. E. Koonin, D. J. Dean, and K. Langanke, Phys. Rep. **278**, 1 (1997), and references therein.
[6] T. Otsuka and T. Mizusaki, J. Phys. G **25**, 699 (1999).
[7] D. C. Zheng, B. R. Barrett, J. P. Vary, W. C. Haxton, and C.-L. Song, Phys. Rev. C **52**, 2488 (1995).
[8] W. C. Haxton and C.-L. Song, in *Nuclear Physics with Effective Field Theory*, edited by P. Bedaque *et al.* (World Scientific, Singapore, 2000), p. 317.
[9] C. Bloch and J. Horowitz, Nucl. Phys. **8**, 91 (1958).
[10] B. R. Barrett and M. W. Kirson, in *Advances in Nuclear Physics*, edited by M. Baranger and E. Vogt (Plenum, New York, 1973), Vol. 6, p. 219.
[11] T. T. S. Kuo and E. Osnes, *Lecture Notes in Physics*, edited by H. Araki *et al.* (Springer-Verlag, Berlin, 1990), Vol. 364.
[12] T. H. Shucan and H. A. Weidenmuller, Ann. Phys. (N.Y.) **73**, 108 (1972); **76**, 483 (1973).
[13] R. Haydock, J. Phys. A **7**, 2120 (1974).
[14] C.-L. Song, Ph.D. thesis, University of Washington, 1998 (available from WCH).
[15] M. Moshinsky, *The Harmonic Oscillator in Modern Physics* (Gordon and Breach, New York, 1969).