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HEAVY ION PHYSICS

Nuclear Physics from Scratch

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Abstract. We report on applications of the *ab initio*, no-core shell model with the primary goal of achieving an accurate description of nuclear structure and reactions from the fundamental inter-nucleon interactions. We show that realistic two-nucleon interactions are inadequate to describe the low-lying structure of ^{10}B, and that realistic three-nucleon interactions are essential. We report preliminary attempts to compute astrophysical S-factors

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1. Introduction

A long-standing goal in nuclear physics is to arrive at a complete and fundamental understanding of nuclear phenomena, in particular, their structure and their reactions. Our principal goal is to determine if our knowledge of the fundamental interaction between pairs of nucleons is sufficient to describe the rich and complex structure observed in nuclei. This is an extremely difficult enterprise, and substantial progress towards this end has been accomplished in the last five years or so. In general, the lightest nuclei, with four or fewer nucleons, are amenable to exact methods based on Faddeev-like [1,2] approaches. The hyperspherical formalism [3,4] has also been applied to three- and four-body systems, with convergence towards exact results being achievable. For heavier nuclei, two methods have proven to be successful so far. Perhaps, the gold standard is Green's Function Monte Carlo [5,6], which has been extensively applied to systems up to ten nucleons [7], and recently ^{12}C. The second method, which we will focus on here, is the *ab initio*, No-core Shell Model (NCSM) [8,9]. The NCSM is a basis-state expansion approach where the interaction between the many-body basis states is derived from fundamental

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inter-nucleon interactions using effective interaction theory. Here, we outline efforts underway at Livermore to apply the No-core Shell Model to the nuclear many-body problem.

2. Effective Interactions and the Shell Model

The basic task at hand is to obtain solutions to the standard eigenvalue problem

$$(\hat{H} - E_\nu)\Psi_\nu = 0\,, \tag{1}$$

where E_ν is the desired eigenvalue, $\hat{H}$ is the Hamiltonian, and Ψ_ν is the eigenfunction. One starting point for solving Eq. (1) is the interacting shell model [10], where we introduce a set of orthogonal basis states ϕ_i to construct the exact solution, i.e. $\Psi_\nu = \sum_i c_{\nu i}\phi_i$. Solutions to Eq. (1) can then be obtained from a set of coupled equations that can be solved using matrix diagonalization techniques. The primary difficulty encountered is that because of the short-range repulsion in the nucleon–nucleon interaction, a basis of infinite dimension is required.

This infinite basis problem can, in principle, be circumvented by the use of effective-interaction theory. First, one chooses manageable subset of the original basis states, which is defined by the operator $\hat{P}$, leading to the slightly different eigenvalue problem

$$(\hat{H}_{\rm eff} - E_\nu)\hat{P}\Psi_\nu = 0\,, \tag{2}$$

where $\hat{P}\Psi_\nu$ is the projection of the exact solution onto the chosen model space, E_ν is again the eigenvalue, and $\hat{H}_{\rm eff}$ is an effective Hamiltonian that yields the *exact* solution of Eq. (1). The excluded space is then usually defined by the operator $\hat{Q}$, with $\hat{P} + \hat{Q} = 1$, $\hat{P}^2 = \hat{P}$, $\hat{Q}^2 = \hat{Q}$, and $\hat{P}\hat{Q} = \hat{Q}\hat{P} = 0$.

An important feature of $\hat{H}_{\rm eff}$ is that it is composed of two-, three-, ..., A-body components even if the fundamental interaction is only pair-wise. The power of $H_{\rm eff}$ is that it may provide a mechanism to carry out computationally tractable calculations while including the relevant physics. For most potentials, the dominant correlations in the effective interactions are at the two-body level, but for smaller P-space, the higher-body correlations are essential for a correct result.

Here, we utilized a unitary transformation due to Lee and Suzuki [11] to derive the effective interaction. This formalism is the foundation for the highly successful no-core shell model (NCSM) [8, 9]. The procedure is based on finding the transformation, e^S, to the Hamiltonian so that the P- and Q-spaces for the many-body problem are decoupled, i.e.

$$\hat{Q}e^{-S}\hat{H}e^{S}\hat{P} = 0\,. \tag{3}$$

Strictly speaking, in this form, $\hat{H}_{\rm eff}$ is not unitary, but can be made so. Explicit formulae for the n-body matrix elements are given by Eqs. (9) and (10) in Ref. [9].

Our calculations begin with the two-body and three-body Hamiltonian for the A-nucleon system, which depends on the intrinsic coordinates alone. We utilize realistic interaction potentials that are derived from nucleon–nucleon scattering

data. To facilitate our calculations, we introduce an A-nucleon harmonic-oscillator Hamiltonian acting only on the center-of-mass, whose effect is subtracted from the many-body calculation. The primary advantages of the harmonic oscillator are that it acts as pseudo mean field providing a convenient basis for expanding the many-body wave function and that the relative motion of the center-of-mass can be separated from the intrinsic degrees of freedom exactly. Within the harmonic-oscillator basis, we specify the P-space, designated by the maximum number, $N_{\max}$, of oscillator quanta excitations, and construct the A-body basis. We then obtain the eigenvalues, E_ν, using a shell-model code. This amounts to diagonalizing a symmetric matrix, whose dimensions are given by the number of A-body basis states. Although the dimensions can be quite large, efficient numerical techniques, such as Lanczos [12], exist that yield the lowest eigenvalues. The parameters governing convergence are: $N_{\max}$, defining the model space; n, the number of clusters in the effective interaction; and $b = \sqrt{m\Omega/\hbar}$, the oscillator parameter setting the physical scale. Ideally, once convergence is achieved, the NCSM solution is independent of these parameters. In practice, the best solution is taken for the largest $N_{\max}$ that is computationally feasible and a value of the oscillator parameter where the binding energy is least sensitive.

Generally, computational limitations impose a compromise in the choice of $N_{\max}$ and $\hat{H}^{(n)}_{\rm eff}$. This is due to the fact that for each increment in $N_{\max}$ or n the computational requirements increase dramatically. Furthermore, the effective interaction itself becomes more difficult to evaluate with increasing n and/or $N_{\max}$. To illustrate the level complexity of the three-body calculations, for $N_{\max} = 4$, 39,523,066 3-particle interaction matrix elements are needed. In this space, the number of M-scheme 10-body configurations for ^{10}B with $J^\pi_z = 0^+$ is 581,740, and the resultant matrix to be diagonalized has over 2.2×10^9 non-zero elements.

3. Nuclear Structure Calculations

Over the past several years, extensive studies have been performed with the NCSM using realistic NN interactions such as the Argonne AV8′ potentials [6] and CD-Bonn [13]. These include first the *ab initio* applications [14] for ^{12}C, $A = 6$ nuclei [15], an examination of the nature of excited states in ^{8}Be, large-basis applications for $A = 10$ nuclei [17], and a study of parity inversion in $A = 11$ nuclei [18]. The study with $A = 6$ provides an excellent example of the convergence and the utility of the no-core shell model [15]. In particular, in Fig. 1, we compare the NCSM spectrum for ^{6}Li (as a function of the model space $N_{\max}$) using the Argonne AV8′ potential with results obtained from the GFMC method. Overall, there is good agreement between the two methods.

Higher-body clusters generally improve the overall convergence [19] of the NCSM. Binding energies for ^{6}Li, ^{8}Be, and ^{10}B are shown in Fig. 2. On the left side of the figure the binding energies are plotted as a function of the oscillator parameter. The figure shows parabolas for the various model spaces (denoted by the $N_{\max}$ value)

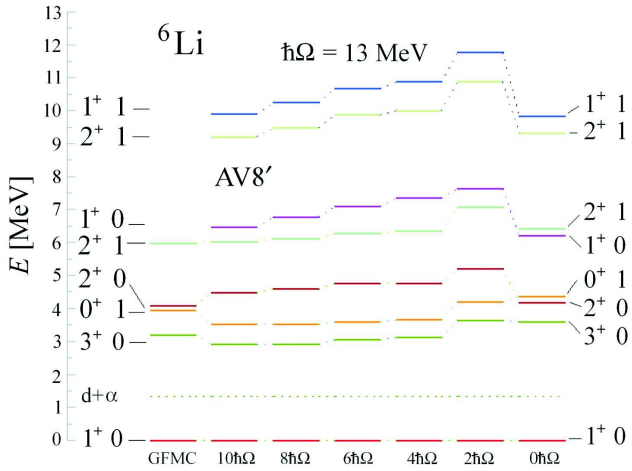

Fig. 1. Comparison of the NCSM and GFMC spectra obtained for the Argonne AV8′ potential. The NCSM spectra are shown as a function of the model size denoted by $N_{\max}\hbar\Omega$

for two-body ($V_{2\text{eff}}$ – dotted lines) and three-body ($V_{3\text{eff}}$ – solid lines) effective interactions. The behavior on the oscillator parameter is lessened (flatter parabola) as either the model space size increases or when more clusters are included in the effective interaction. Again, the "best" result for a given model space is chosen in the region exhibiting the least dependence on the oscillator parameter. These "best" values are plotted on the right side of the figure as a function of the model space $N_{\max}$ and compared with the results from the GFMC method (full solid lines with a dotted line band denoting the GFMC uncertainty). For a given value of $N_{\max}$, faster convergence is achieved with higher clusters in H_{eff}. In addition, we note that the NCSM calculation with the two-body effective interaction still differs from the GFMC result by ≈1.8 MeV even for the largest model space. On the other hand, the three-body effective interaction results are in better agreement for smaller model spaces. Given that ^{8}Be is actually an unbound alpha cluster, this suggests that the three-body effective interactions includes more correlations. Overall, the results obtained with the three-body clusters in the effective interaction are in agreement with the GFMC calculations to within 400 keV.

With confidence in convergence, we now turn to a study of the structure of light nuclei. A particularly salient example is ^{10}B. The spectrum obtained with the AV8′ is shown in Fig. 3 (using a three-body effective interaction, $V_{3\text{eff}}$) in comparison with experiment. We note that the ground state (3^+) and the first excited state (1^+) are reversed in order. This behavior is a feature that is common to all the realistic nucleon–nucleon forces, and is the first direct evidence that, in addition to providing extra binding, the three-nucleon forces is important for determining nuclear structure.

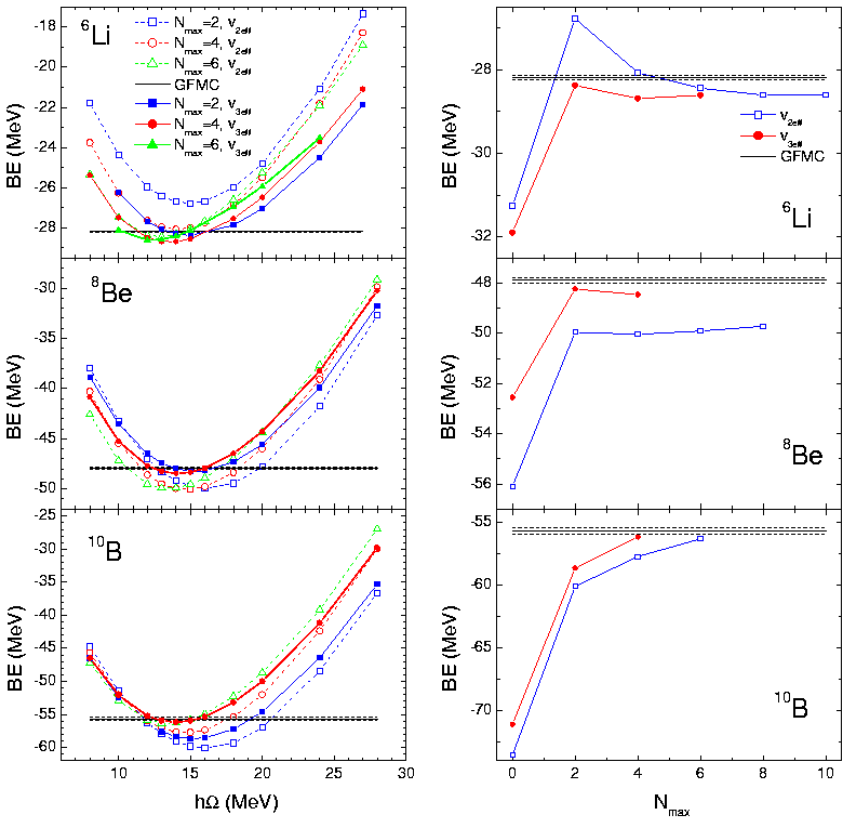

Fig. 2. Calculated ground-state energy of ^{6}Li (upper panel), ^{8}Be (middle panel) and ^{10}B (lower panel) using the AV8′ *NN* potential with Coulomb. Results using the two-body effective interaction and the three-body effective interaction in basis spaces up to $6\hbar\Omega$ in the range of HO frequencies of $\hbar\Omega$ = 8–28 MeV are shown and compared to the GFMC results from Ref. [6]. On the rhs, the energies at the HO frequency minima as a function of $N_{\max}$ are plotted

We conclude that we must now include "true" three-nucleon forces. These are different from the three-body clusters in the effective interaction, which are induced because of the effect of the finite model space. We have carried out calculations including the Tucson–Melbourne three-nucleon force [20] for ^{10}B, and the results are shown in Fig. 3, where better agreement with the experimental spectrum is obtained, In particular, the ordering of the first two states is now correct. Overall, one finds that the three-nucleon interaction has spin-orbit components that play an important role in determining the structure of light p-shell nuclei. We have also demonstrated that certain transition operators, such as Gamow–Teller and M1, are also strongly affected by the three-nucleon interaction. This is due to the presence of strong spin-orbit components in the three-nucleon interaction. A simple explanation is that

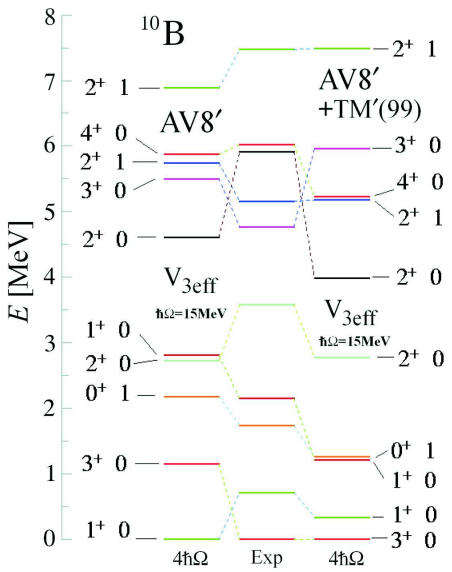

Fig. 3. Comparison of low-lying spectrum of ^{10}B obtained with the AV8′ two-nucleon interaction alone (left side) and with the Tucson–Melbourne three-nucleon force (right side) with experiment

without a strong spin-orbit component the nuclear Hamiltonian is nearly invariant to the group SU(4). Given that the Gamow–Teller transition operator is a generator of SU(4), it cannot mediate transitions between different SU(4) irreps, which would lead to a significant suppression of Gamow–Teller transition amplitudes. The spin-orbit components in the three-nucleon force, however, break SU(4) symmetry, and, hence, lead to much larger Gamow–Teller and M1 matrix elements. All this points to the fact that we must include realistic three-nucleon forces for a proper description of the properties of nuclei.

4. Reactions

In addition to an *ab initio* description of structure, we would also like to have a theoretical description of reactions that is based on the fundamental inter-nucleon interactions. Of particular interest are the light-ion fusion reactions that characterize stellar evolution. We are in the process of extending the No-core Shell Model into a formalism to describe reactions with binary entrance and exit channels.

The starting point for our formalism is the *ab initio* solution to the composite nucleus with A nucleons, and the projectile and target with a and $A-a$ nucleons, respectively. Naturally, we also require solutions for binary exit clusters as well. In the asymptotic region, the A-nucleon wave function is given by the product of the binary intrinsic wave functions coupled to asymptotic channel quantum numbers and a radial wave function representing their relative motion

$$|\Phi^{JM}_{A-a\alpha I_1,a\beta I_2,sl};g\rangle \quad = \quad \sum (I_1 M_1 I_2 M_2|sm_s)|A-a,\alpha I_1 M_1\rangle|a,\beta I_2 M_2\rangle$$

$$(sm_s lm_l|JM)Y_{lm_l}(\hat{r})g^J_{A-a\alpha I_1,a\beta I_2,sl}(r)\,, \tag{4}$$

where $|A-a,\alpha I_1 M_1\rangle$ and $|a,\beta I_2 M_2\rangle$ are eigenstates of $\hat{H}^{A-a}_{\rm eff}$ and $\hat{H}^{a}_{\rm eff}$, respectively, and describe the internal states of the two clusters. Here, the intrinsic angular momenta I_1 and I_2 are coupled to the channel spin s, which in turn is coupled to the channel orbital angular momentum l to the total angular momentum J. The relative coordinate $\vec{r}$ measures the separation of the center-of-mass of the two clusters. The radial wave function g describes the relative motion of the clusters. The asymptotic behavior of the radial wave functions determines the reaction cross sections. A key ingredient for the formalism is the radial cluster form factor, given by the overlap

$$\langle A\lambda J|\mathcal{A}\Phi^{JM}_{A-a\alpha I_1,a\beta I_2,sl};\delta(r)\rangle, \tag{5}$$

which measures the overlap of the composite A-body system with the a- and $(A-a)$-body clusters as a function of their separation r. Here $\mathcal{A}$ denotes the antisymmetrization operation.

With the calculated radial-cluster form factors, proper antisymmetrization, a suitable renormalization of the radial wave function overlaps, and considerable algebra, we arrive at a set of coupled integro-differential equations for $u(r)=g(r)/r$, which embody much of the physics of formalism, and determine the reaction cross section. Specifically,

$$\left[-\frac{\hbar^2}{2M_{\rm red}}\frac{d^2}{dr^2_{A-a}}+\frac{\hbar^2}{2M_{\rm red}}\frac{l(l+1)}{r^2_{A-a}}+V_{\rm Fold}(r)+E^{A-a}_{\alpha,I_1}+E^{a}_{\beta,I_2}-E\right]u^J_{\Gamma(\Gamma_i)}(r_{A-a})$$
$$+\sum_{\Gamma' nn'}\int_0^\infty dr'_{A-a}R_{nl}(r_{A-a})\mathcal{H}^J_{\Gamma n,\Gamma' n'}R_{n'l'}(r'_{A-a})u^J_{\Gamma'(\Gamma_i)}(r'_{A-a})=0\,,$$

where $V_{\rm Fold}$ is an optical model-like potential derived from the effective Hamiltonian and includes the Coulomb potential. Other quantities in Eq. (6) are: r_{A-a} the relative coordinate for the channel with $A-a$ and a clusters, $M_{\rm red}=M_n(A-a)\,a/A$ (M_n is the nucleon mass), E^{A-a}_{α,I_1} and E^{a}_{β,I_2} are the energies of the intrinsic states for the clusters (i.e. eigenstates of $\hat{H}^{A-a(a)}_{\rm eff}$), respectively, E is the total energy of the A-body system. The labels Γ are short-hand for the channel state labels $(A-a)\,\alpha I_1, a\beta I_2, sl$, with Γ_i referring to the entrance channel for the reaction. The sum over Γ denotes an explicit sum over all final channels, including different $(A-a,a)$ combinations. The matrix elements $\mathcal{H}_{\Gamma n,\Gamma' n'}$ are calculated using the effective Hamiltonian and the asymptotic wave functions for each channel as defined in Eq. (4) (with g replaced by the radial HO wave function R_{nl}), and, thus are explicit functions of the radial-cluster form factor. The asymptotic boundary condition is obtained by matching the radial wave functions g to the correct asymptotic behavior. The reaction cross section for each channel is then determined from the amplitudes of the asymptotic components of the channel relative wave functions.

At present much work is still left to formally solve the equation of motion, and hence obtain the cross section. We have developed codes to compute the

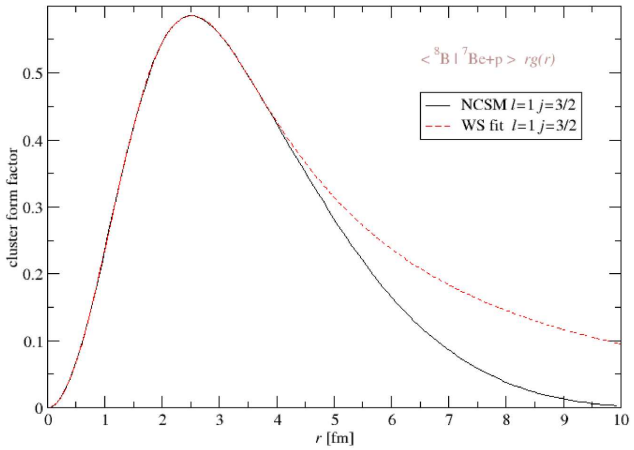

Fig. 4. Computed radial-cluster form factor, $rg(r)$, for the ground state of ^{7}Be plus proton with the ground state of ^{8}B. The solid line represents the NCSM result, while the dashed line represents a renormalized overlap obtained from a Woods–Saxon potential whose parameters were fit to the compute overlap up to 3.5 fm and constraining the energy to reproduce the experimental separation energy

radial-cluster form factor and have preliminary evaluations of the S-factor for the ^{7}Be(p,γ)^{8}B reaction. Shown in Fig. 4 is the calculated cluster form factor ^{7}Be+p

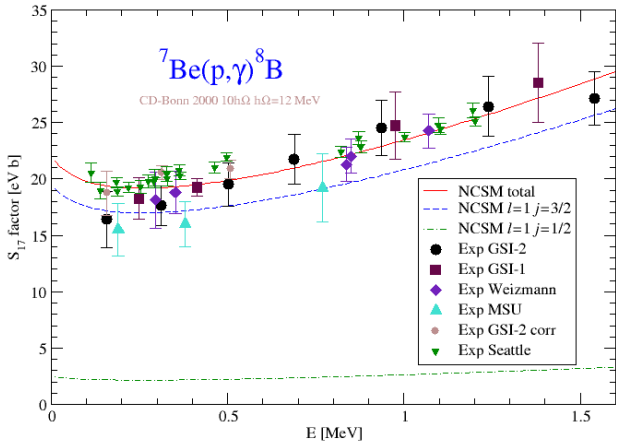

Fig. 5. Preliminary calculation of the ^{7}Be(p,γ)^{8}B S-factor using renormalized cluster form factors as shown in Fig. 4. The dashed and dashed–dotted lines show the contribution due to the $l = 1$, $j = 3/2$ and $j = 1/2$ states, respectively

(black line). Note that the integral of the squared overlap is the spectroscopic factor. The first feature to note is that because we utilize a harmonic-oscillator basis, the radial wave function has the wrong asymptotic behavior, as it decays as a Gaussian. This can be corrected considerably with effective operators, and is under development. We can obtain a quick solution to this problem by using a wave function obtained with a Woods–Saxon potential. Here we fit a Woods–Saxon potential to the computed overlap up to 3.5 fm or so, and require that energy of the state reproduce the experimental separation energy. This is denoted by the red line in Fig. 4. We then renormalize the magnitude of the overlap to preserve the spectroscopic factor. Using these radial-cluster form factors, we then preliminarily compute the S-factor for ^{7}Be(p,γ)^{8}B with the radiative capture model of Bertulani [21], which is shown in Fig. 5. Overall, good agreement with the current experimental data is achieved, suggesting that our full formalism has the potential to provide the capability to yield an exact computation of reactions, including astrophysical S-factors, with the fundamental interactions between nucleons.

5. Conclusions

Substantial progress has been made towards an exact description of nuclear structure. In this work, we describe the *ab initio*, No-core Shell Model and recent results. In particular, we find that realistic *NN* interactions by themselves are inadequate and that three-nucleon forces play an important role in determining nuclear properties. We are also in the process of extending the No-core Shell Model into a formalism capable of providing an exact description of nuclear reactions. Overall, the prospects are bright that exact results for both structure and reactions for nuclei up to Oxygen utilizing the fundamental forces between nucleons can be achieved in the near future.

Acknowledgments

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