Large-space shell-model calculations for light nuclei

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An effective two-body interaction is constructed from a new Reid-like NN potential for a large no-core space consisting of six major shells and is used to generate the shell-model properties for light nuclei from $A=2$ to 6. For practical reasons, the model space is partially truncated for $A=6$. Binding energies and other physical observables are calculated and they compare favorably with experiment.

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I. INTRODUCTION

In traditional nuclear shell-model calculations, only a few particles or holes with respect to a closed shell are treated as active within a restricted model space. In a well-studied example, ^{18}O, the model space contains one major shell, the $1s$-$0d$ shell, with two valence nucleons. These calculations require effective-interaction matrix elements along with calculated or empirical single-particle (SP) energies as input. The effective interaction could either be "phenomenological" (see, for example, Refs. [1–3]) or "realistic"(see, for example, Refs. [4, 5]), depending on how it is obtained. Both types of effective interactions have been substantially used with success, when good agreement with experimental spectra is taken as the criterion. A phenomenological interaction might be obtained by fitting selected energy spectra and electromagnetic properties of the nuclei in the region of interest.

In the case of a realistic interaction, which is our main concern in this work, one usually starts with the Brueckner reaction matrix G [6] (i.e., ladder diagrams) calculated from a realistic nucleon-nucleon (NN) potential for a specified model space, and evaluates other diagrams (e.g., folded diagrams and/or core-polarization diagrams [7]) using the G matrix. This renormalization procedure is incomplete, however, because so far, the core-polarization diagrams can only be included to, at most, third order in the perturbation-theory expansion [8–10]. The incompleteness here presents a serious problem because convergence has not been attained within the lowest few orders of the perturbation expansion [8, 11]. Similar uncertainties exist when calculating the effective operators [7] to be used in the model space.

Recently, attempts [12–17] have been made to avoid the above difficulty by adopting a no-core model space in which all nucleons in a nucleus are treated as active. It is considerably simpler to obtain the effective interaction for a no-core space since there are no hole lines and the complicated core-polarization processes are absent. Consequently, one is left with the ladder diagrams and the folded diagrams for the effective interaction which may include effective many-body contributions.

Within the concept of no-core calculations, it is im-

portant to distinguish two cases. In the case we call a "full" no-core calculation, one selects a set of d model-space SP states and then generates the configurations where all nucleons can occupy all orbitals in all possible, Pauli-allowed, ways. In an "$N_{max}\hbar\Omega$ truncated" no-core calculation, only those configurations are retained from the full no-core case in which there are up to and including $N_{max}\hbar\Omega$ excitations of the lowest unperturbed configuration (in harmonic oscillator notation) of the A nucleons.

To be more specific, let us consider a $2\hbar\Omega$ (i.e., $N_{max}=2$) shell-model diagonalization for ^{6}Li in a no-core model space consisting of the lowest four major shells ($0s$, $0p$, $1s$-$0d$, and $1p$-$0f$). In this case, the configuration with a hole in the $0s_{\frac{1}{2}}$ shell and a particle in the $1s$-$0d$ shell [i.e., $(0s)^3(0p)^2(1s0d)^1$] is allowed. The configuration [i.e., $(0s)^2(0p)^4$] is also taken into account. However, one cannot claim to have performed a "full" no-core calculation because only one or two, out of four, $0s$ nucleons are allowed to be excited to the higher shells. Namely, in this $2\hbar\Omega$ truncated calculation, not all nucleons are active, and there still is a partially inert core.

On the other hand, if one includes $2s$-$1d$-$0g$ and $2p$-$1f$-$0h$ major shells and performs a $4\hbar\Omega$ calculation for the same nucleus, the configuration $(0p)^6$ will be allowed, leaving no nucleons in the "core" orbital $0s_{\frac{1}{2}}$. Although such a calculation is still restricted, it is surely more complete than the $2\hbar\Omega$ calculation. It is not currently possible to actually carry out a full no-core calculation in many cases we want to investigate. Our hope is that as N_{max} increases, the results will converge and approach those of the full no-core calculation.

Another practical issue of working with an $N_{max}\hbar\Omega$ truncated no-core calculation is that this facilitates the accurate treatment of the spurious center-of-mass (c.m.) motion. If $(N_0 + 1)\hbar\Omega$ is defined as the minimum SP excitation energy needed to lift a nucleon to the lowest unperturbed state outside the model space ($N_0=4$ for the ^{6}Li example above in the model space through the $2p$-$1f$-$0h$ shell), then, for $N_{max} = N_0$, it is possible to obtain no-core shell-model wave functions free of spurious c.m. motion.

It is an ultimate goal of the nuclear shell model to be able to start with a realistic NN potential and obtain

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unambiguous and converged results against the changes in the size of the model space and in the choice of the unperturbed basis. Convergence with model-space size means convergence with increasing N_{max} and increasing d, a dual convergence criterion.

Encouraging results have been obtained recently for very light nuclei in Ref. [18], by Ceuleneer et al. They have performed a shell-model calculation for the $T=0$ states in ^{4}He, where up to $10\hbar\Omega$ excitations from the basic configuration $[(0s_{\frac{1}{2}})^4]$ are allowed. The only input to the calculation is a set of two-body matrix elements (TBME's) of a modified Sussex interaction. Since this effective interaction does not have a theoretically derived model-space dependence, they multiplied all two-body matrix elements by a model-space-dependent parameter which is adjusted to get the correct binding energy. The step of deriving the dependence of this parameter on the model-space size is now required to complete the dual convergence test.

In this work, we will adopt a large no-core harmonic-oscillator (HO) model space consisting of six major shells (from $0s$ to $2p$-$1f$-$0h$). We will consider several light nuclei ranging from $A=2$ to $A=6$. An effective interaction will be constructed for the above model space from a new Reid-like NN potential (denoted by Reid93) provided by the Nijmegen group [19]. Note that we will use effective interactions constructed in exactly the same manner for all the nuclei considered here. We will follow an approach that favors the more accurate treatment of the spurious c.m. motion and attempts to minimize the neglect to the two-body "ladder" scattering procedures. We have designed an even more accurate approach along these lines which involves excitation-dependent effective interactions and will be reported in a future work [20].

It is an established fact that for a small model space, a mass-dependent two-body effective interaction gives an overall better description [2, 21]. But we anticipate that such a mass dependence will become weaker as the size of the no-core model space is increased. Similarly, we expect the effective many-body forces to decrease with an increasing model space. Indeed, if an infinitely large model space is used, the effective interaction reverts back to the NN potential v, whose matrix elements are clearly independent of the nucleus under consideration. Throughout the remainder of this work, we assume that the model space is sufficiently large and the SP basis is sufficiently realistic that we can neglect the effective many-body interactions. This will be investigated in a future effort, which also addresses the rate our methods approach the goal of satisfying the dual convergence criteria.

II. EFFECTIVE INTERACTION

For a no-core model space, the core-polarization diagrams are not present, and the two-body effective interaction is simply the G matrix [6] plus the folded diagrams series [22]. The G matrix is the sum of the ladder diagram series which represents the multiple scattering processes of two nucleons in a nuclear medium. We continue to follow our philosophy given in Ref. [17] for the no-core G

matrix in large spaces which treats two-particle scattering via a realistic NN interaction v_{12} in an "external" field u, which is provided by the other nucleons in the same nucleus. Thus, we write

$$G(\omega) = v_{12} + v_{12}\frac{Q}{\omega - (h_1 + h_2)}G(\omega)$$
$$= v_{12} + v_{12}\frac{Q}{\omega - (h_1 + h_2 + v_{12})}v_{12}, \qquad (1)$$

where $h = t + u$ is the one-body Hamiltonian and u is the nuclear mean field. The quantity ω is the starting energy, which represents the initial energy of the two in-medium nucleons. The Pauli operator Q excludes the scattering of the two nucleons into the intermediate states which are inside the model space. It is therefore related to the choice of the model space and will be specified in the next section.

A rigid prescription for the nuclear mean field u is not necessary since the results will be independent of u once the dual convergence criteria are satisfied. In most practical calculations, u is approximated by a one-body potential of a simple and convenient form. The two most common choices for u are a shifted HO potential and zero:

$$u(r) = -V_0 + \frac{1}{2}m\Omega^2r^2, \qquad (2)$$
$$u(r) = 0. \qquad (3)$$

The latter choice corresponds to a plane-wave basis. Some hybrid approaches have been developed which use oscillator states for low-lying orbitals and plane waves, orthogonalized to the oscillator states, for all the remaining states [23, 24].

Although a shifted HO potential (2) does not have the expected asymptotic behavior of vanishing exponentially at large r, it was argued in Ref. [17] that the shape of the assumed u at large r might not be very important since, except for some weakly bound states, nucleons are unlikely to move far beyond the nuclear mass radius.

One may further notice from Refs. [4, 25] that the two seemingly very different one-body potentials in Eqs. (2), (3) actually led to rather similar G-matrix elements, provided one makes a careful choice for the starting energy (related to the choice of u). Note that the constant shift V_0 in Eq. (2) is more a matter of convenience, as a shift of $2V_0$ can be made in the starting energy ω in Eq. (1), i.e.,

$$\omega = \omega' - 2V_0, \qquad (4)$$

to cancel out V_0 in the energy denominator [17].

In this work, we will approximate the nuclear mean field by the HO potential (2) not only because this simplifies the G-matrix calculation [25, 26], but, more importantly, for the reason that this makes possible an exact removal of the effects of the spurious c.m. motion from our many-body wave functions. Once the G matrix $G(\omega)$ is obtained as a function of the starting energy, it will not be difficult to evaluate the folded diagrams using the techniques developed by Kuo and Krenciglowa [27] and by Lee and Suzuki [28] and to obtain a starting-energy-

independent effective two-body interaction (denoted by $v_{\text{eff}}^{(2)}$).

One must bear in mind that $v_{\text{eff}}^{(2)}$ obtained in this procedure depends on the assumption made for the one-body potential in the G-matrix calculation. Especially in cases when the model spaces are small and we are further from satisfying the dual convergence criteria, it is important to use a u that sensibly represents the nuclear mean field so as to minimize the neglected many-body interactions [29] and higher than linear order "$-u$" insertions.

In Ref. [17] it is shown that $v_{\text{eff}}^{(2)}$ can be well approximated by the G matrix calculated at starting energies which are related to the initial unperturbed energy of the two nucleons in the ladder scattering processes in a simple way:

$$\omega' = \omega + 2V_0 = \epsilon_a + \epsilon_b + \Delta, \tag{5}$$

where $\epsilon = (2n_r + l + 3/2)\hbar\Omega$ are the HO SP energies (a and b are the SP states that the two nucleons initially occupy). Such a state-dependent choice for ω' will lead to a non-Hermitian G matrix, but the non-Hermiticity is found to be small. The quantity Δ signifies the interaction energy between the two nucleons. In a specific application to ^{6}Li, it has been shown [17] that for $\hbar\Omega=18$ MeV, a value of -21 MeV for Δ results in $G(\omega')$ which is an excellent approximation to $v_{\text{eff}}^{(2)}$. However, it is also observed in Ref. [17] that $v_{\text{eff}}^{(2)}$ calculated for a smaller value of $\hbar\Omega$ (e.g., 14 MeV) tends to overbind ^{4}He and ^{6}Li. In a more recent investigation [30], it is further concluded that the overbinding problem arises from non-negligible, many-body folded diagrams. Since it is rather involved to evaluate effective many-body forces, in general, and many-body folded diagrams, in particular, we will omit all folded diagrams from the present calculations.

We, therefore, adopt the average of $G(\omega')$ and its Hermitian conjugate, calculated for a HO basis with $\hbar\Omega=14$ MeV and ω' given by Eq. (5), as the effective interaction. But the parameter Δ is not chosen to best approximate $v_{\text{eff}}^{(2)}$ (which will lead to overbinding if the effective

many-body forces are not included); rather, it is chosen to yield the experimental binding energy. Initially, one might expect that different values of Δ have to be used for different nuclei. But, quite surprisingly, we find that good agreement with experimental observables can be obtained with a nucleus-independent value of Δ (-35 MeV). Results obtained with different choices of $\hbar\Omega$ and Δ will be discussed in Sec. III E.

Our shell-model Hamiltonian will now be written as

$$H_{\text{SM}} = \left(\sum_{i=1}^{A} t_i - T_{\text{c.m.}}\right) + \sum_{i<j}^{A} G_{ij} + V_{\text{Coulomb}}$$
$$+ \lambda\left(H_{\text{c.m.}} - \frac{3}{2}\hbar\Omega\right), \tag{6}$$

where $t_i = \mathbf{p}_i^2/(2m)$ are the one-body kinetic energies, $T_{\text{c.m.}} = (\sum_i \mathbf{p}_i)^2/(2mA)$ the c.m. kinetic energy, and V_{Coulomb} the Coulomb interaction. The proton and neutron masses are taken to be the same. The last term (with $\lambda=10$) in the above equation forces the c.m. motion of the low-lying states in the calculated spectrum to be in its lowest HO configuration.

We remark that our calculations involve no free parameters other than those used in calculating the G matrix, $\hbar\Omega$ and Δ. Moreover, these two parameters are fixed at 14 MeV and -35 MeV, respectively, for all nuclei considered in the present work.

We emphasize that in a no-core calculation, we are attempting to derive all shell-model properties from an underlying Hamiltonian H_{SM}. Thus, there are no phenomenological SP energy terms in H_{SM}.

III. RESULTS AND DISCUSSION

As previously mentioned, we use a no-core model space containing the lowest six HO major shells with $\hbar\Omega=14$ MeV. For $A \leq 4$, we allow all $0\hbar\Omega$–$7\hbar\Omega$ configurations within the model space. For $A > 4$, we allow all $0\hbar\Omega$–$5\hbar\Omega$ configurations. Therefore, different Q operators have to be used in Eq. (1) for $A \leq 4$ and $A > 4$:

for $A \leq 4$: $Q = 1$ for $n_1 \geq 6$, $n_2 \geq 6$, or $n_1 + n_2 \geq 8$, $\qquad$ (7)

$\qquad\qquad\qquad = 0$ otherwise;

for $A > 4$: $Q = 1$ for $n_1 + n_2 \geq 6$, $\qquad\qquad\qquad\qquad\qquad\qquad$ (8)

$\qquad\qquad\qquad = 0$ otherwise.

In the above equations, $n=2n_r+l$ is the principal quantum number for the HO SP states. It starts from 0 with $n=0$ representing the first major shell ($0s$). For $A=6$, due to the computer memory limitation, the $n=5$ shell contains only the p orbitals; the f and h orbitals are left outside the model space.

The shell-model matrix diagonalizations are performed for the Hamiltonian H_{SM} in Eq. (6) using the many-fermion-dynamics code [31]. The results are given in Table I, which we will discuss in the following subsections. The experimental results given in Table I are taken from

Ref. [32] for $A=3$, Ref. [33] for $A=4$, and Ref. [34] for $A=5$ and 6.

A. Binding energies

It is possible to obtain exact or nearly exact results for ground-state energies of the lightest nuclei by solving the Schrödinger or Faddeev [35] equations for realistic NN interactions. This has been done for the ground states of ^{3}H, ^{3}He, and ^{4}He [36–39]. Even for ^{5}He and ^{6}Li, preliminary results obtained by Wiringa in varia-

tional Monte Carlo calculations have appeared [40]. Unlike the few-body approaches in which one obtains almost exact results, at least for the ground state, the effective-interaction shell-model approach involves some uncertainties due to the truncation of the space and the approximation made in calculating the effective interaction for the truncated space. Consequently, the shell-model approach to the above light nuclei, although being able to calculate for a given set of quantum numbers the excited states as easily as the lowest state, cannot match the few-body approach in the accuracy of the results for the ground state. Nevertheless, our ultimate goal is to satisfy the dual covergence criteria. By using a large no-core model space along with a reasonable effective interaction, we hope to demonstrate that, in spite of its

present limitations, the effective Hamiltonian approach gives a useful description of the low-lying states in light nuclei.

Our results are encouraging as can be seen from Table I. The calculated binding energies for the deuteron, triton, ^{4}He, ^{5}He, and ^{6}Li are 2.103, 8.589, 28.757, 25.960, and 30.648 MeV, respectively, agreeing quite well with the corresponding experimental values of 2.225, 8.482, 28.296, 27.410, and 31.996 MeV. Of course, it is more relevant to compare our results to those obtained in the exact few-body approaches using the same potential. These approaches show that existing realistic NN potentials underbind light nuclei with $A > 2$. Our calculations involve a free parameter Δ which has been fixed at -35 MeV for all the nuclei considered. For $A > 2$, we can ob-

TABLE I. The results for ^{2}H, ^{3}H, ^{4}He, ^{5}He, and ^{6}Li obtained in large no-core (consisting of six HO major shells) shell-model calculations. The experimental data are taken from Refs. [32–34]. In the table, E_B is the binding energy (in MeV) and $E_x(J_n^\pi,T)$ the excitation energy (in MeV) of the J_n^π,T state. The ground-state rms $point$ radius for protons $\sqrt{\langle r_p^2\rangle}$ (in fm), electric quadrupole moment Q (in $e\,\mathrm{fm}^2$), and magnetic dipole moment μ (in μ_N) are also listed. The "experimental" $\sqrt{\langle r_p^2\rangle}$ was deduced from the charge rms radius $\sqrt{\langle r_c^2\rangle}$ through (ignoring the neutron charge distribution and other higher-order effects and assuming a proton rms charge radius of 0.81 fm) $\langle r_p^2\rangle = \langle r_c^2\rangle - 0.81^2$.

Observable	Calc.	Expt.	Observable	Calc.	Expt.
Deuteron			**Triton**		
E_B	2.103	2.2246	E_B	8.589	8.4819
$\sqrt{\langle r_p^2\rangle}$	1.653	1.95	$\sqrt{\langle r_p^2\rangle}$	1.573	1.41–1.62
μ	0.857	0.8573	μ	2.659	2.9790
Q	0.242	0.2859	$E_x(\tfrac{5}{2}_1^-,\tfrac12)$	12.716	unbound
$E_x(0_1^+,1)$	3.754	unbound	$E_x(\tfrac{1}{2}_1^-,\tfrac12)$	12.868	unbound
^{4}He			**^{5}He**		
E_B	28.757	28.296	E_B	25.960	27.410
$\sqrt{\langle r_p^2\rangle}$	1.488	1.46	$\sqrt{\langle r_p^2\rangle}$	1.659	
$E_x(0_1^+,0)$	0.000	0.00	μ	-1.864	
$E_x(0_2^+,0)$	26.135	20.21	Q	-0.332	
$E_x(0_1^-,0)$	22.848	21.01	$E_x(\tfrac{3}{2}_1^-,\tfrac12)$	0.000	0.00
$E_x(2_1^-,0)$	24.351	21.84	$E_x(\tfrac{1}{2}_1^-,\tfrac12)$	3.112	4 ± 1
$E_x(2_1^-,1)$	25.739	23.33	$E_x(\tfrac{1}{2}_1^+,\tfrac12)$	7.437	See[a]
$E_x(1_1^-,1)$	26.338	23.64	$E_x(\tfrac{5}{2}_1^+,\tfrac12)$	14.206	See[a]
$E_x(1_1^-,0)$	27.337	24.25	$E_x(\tfrac{3}{2}_1^+,\tfrac12)$	14.439	See[a]
$E_x(0_1^-,1)$	27.418	25.28	$E_x(\tfrac{3}{2}_2^+,\tfrac12)$	20.445	16.75[b]
$E_x(1_2^-,1)$	27.905	25.95	$E_x(\tfrac{3}{2}_2^-,\tfrac12)$	21.499	N/A
^{6}Li			$E_x(\tfrac{1}{2}_2^+,\tfrac12)$	23.563	N/A
E_B	30.648	31.996	$E_x(\tfrac{7}{2}_1^+,\tfrac12)$	23.592	N/A
$\sqrt{\langle r_p^2\rangle}$	2.050	2.38	$E_x(\tfrac{1}{2}_2^-,\tfrac12)$	24.045	N/A
μ	0.851	0.822	$E_x(\tfrac{3}{2}_3^+,\tfrac12)$	24.398	N/A
Q	-0.116	-0.082	$E_x(\tfrac{1}{2}_1^+,\tfrac32)$	25.861	N/A
$E_x(1_1^+,0)$	0.000	0.000	$E_x(\tfrac{1}{2}_3^+,\tfrac12)$	26.240	N/A
$E_x(3_1^+,0)$	2.959	2.186	$E_x(\tfrac{3}{2}_4^+,\tfrac12)$	27.359	N/A
$E_x(0_1^+,1)$	3.607	3.563	$E_x(\tfrac{7}{2}_1^-,\tfrac12)$	27.681	N/A
$E_x(2_1^+,0)$	5.485	4.31			
$E_x(2_1^+,1)$	6.505	5.366			
$E_x(1_2^+,0)$	7.828	5.65			

[a]Low-lying positive-parity states (e.g., a $J^\pi=\tfrac12^+$, $T=\tfrac12$ state at $\sim$5 MeV and $J^\pi=\tfrac32^+$, $T=\tfrac12$ and $J^\pi=\tfrac52^+$, $T=\tfrac12$ states at $\sim$12 MeV) are predicted to exist. See Ref. [34] for more details.

[b]We identify the calculated 20.445 MeV state as the experimental 16.75 MeV state, because the calculated state is dominated by the $(0s)^3(0p)^2$ configuration.

tain smaller binding energies (in better agreement with exact calculations) by decreasing Δ (i.e., making it more negative) since the binding energies decrease monotonically with the decreasing Δ. Our adoption of a Δ value that fits experimental binding energies stems from an assumption that our neglected effective many-body forces and other corrections can largely cancel the neglected (and largely unknown) true many-body forces.

It is worth mentioning that for the two-body system, the deuteron, it is possible to obtain exact results even with the effective-interaction approach [41]. Our present results for the deuteron are not exact due to our neglect of the processes which are higher order in u. Our effective interaction nevertheless gives a reasonable deuteron binding energy. In Sec. III C, we will further show that the deuteron magnetic dipole and electric quadrupole moments also come out well.

B. Excitation spectra

For the deuteron and the triton, we obtain only one bound state in the calculations, agreeing with experiment and with exact calculations. For the deuteron, the lowest state in the continuum is a $J^\pi=0^+$, $T=1$ state, which is unbound by 1.65 MeV (i.e., 3.75 MeV above the ground state). For the triton, the lowest excited state is a $J^\pi=\frac{5}{2}^-$, $T=\frac{1}{2}$ state, unbound by 4.13 MeV. It has a nearly degenerate $J^\pi=\frac{1}{2}^-$, $T=\frac{1}{2}$ state, unbound by 4.28 MeV. The $T=\frac{3}{2}$ states are even higher in energy. Therefore, these results do not support nn, pp, nnn, or ppp bound states.

For ^{4}He, the experimental level sequence of the low-lying negative-parity states is correctly reproduced. The excitation energies are consistently higher than the experimental results [33] by about 2–3 MeV. These results are clearly an improvement over those obtained in our previous study [16]. In that study, the excitation energies of these same states were obtained in a smaller model space, including only four major shells, and were found to be as much as 6 MeV too high when compared with experiment (see Table I in Ref. [16]). The better results we obtain here should be attributed mainly to the larger model space and the improved NN interaction. From a theoretical viewpoint, we have also improved the G matrix by using a state-dependent starting energy of Eq. (5) (rather than at a constant starting energy as in Ref. [16]) which better approximates the full effective interaction [17].

We obtain the first excited state ($J^\pi=0^+$, $T=0$) in ^{4}He at an excitation energy of 26.135 MeV. This is about 6 MeV higher than experiment but it is about 7.7 MeV lower than the previous result (33.807 MeV) for the four-major-shell space [16]. Again, the larger model space used in this work is largely responsible for the decrease in energy. A more accurate description of this state will require an even larger space. Indeed, in Ref. [18], where a modified Sussex interaction is used, excellent agreement with experiment is obtained for this state only when up to $10\hbar\Omega$ configurations are included.

The calculated ground state in ^{4}He is dominated by

the $(0s)^4$ configuration but it has a considerable amount of "1p-1h" configuration $(0s)^3(1s)^1$ and "2p-2h" configuration $(0s)^2(0p)^2$. The 0_2^+ state is dominated by the $(0s)^3(1s)^1$ configuration while the $(0s)^2(0p)^2$ and $(0s)^4$ components are also quite significant.

The occupancies of the various model-space orbitals in the 0_1^+ and 0_2^+ states are

$$|^4\text{He}:0_1^+\rangle = (0s)^{3.525}(0p)^{0.160}(sd)^{0.200}(\text{other shells})^{0.114},$$
(9)

$$|^4\text{He}:0_2^+\rangle = (0s)^{2.679}(0p)^{0.521}(sd)^{0.716}(\text{other shells})^{0.084}.$$
(10)

Relative to the ground state, the 0_2^+ state has only about 50% of the "breathing mode" $(0s)^{-1}(1s)^1$. However, this result depends on the choice of the SP basis. If, for example, a Hartree-Fock (HF) basis were used, the oscillator-basis s states would mix to produce the HF s states (e.g., $0s_{\text{HF}}$ and $1s_{\text{HF}}$, etc.) so that the admixture of the $(0s_{\text{HF}})^3(1s_{\text{HF}})^1$ component in the ground state would likely be much smaller. This would lead to a larger amount of $(0s_{\text{HF}})^{-1}(1s_{\text{HF}})^1$ in the 0_2^+ state.

Note that although our model space is not sufficiently large to reproduce the first excited 0^+ state in ^{4}He at the experimental energy, it does a fairly good job for the "$1\hbar\Omega$" states. This gives us confidence in the results for the low-lying states in ^{5}He, which we present below.

The first excited state in ^{5}He ($J^\pi=\frac{1}{2}^-$, $T=\frac{1}{2}$) is obtained at an energy of 3.112 MeV, within the range of 3–5 MeV given in Ref. [34]. The low-lying positive-parity states are also of interest. Experimentally, there is a famous $J^\pi=\frac{3}{2}^+$ state at 16.75 MeV. It has a dominant $(0s)^3(0p)^2$ configuration and can be thought of as the ground state of ^{6}Li coupled to a $0s$ hole. This state corresponds to our calculated 20.445 MeV state in Table I, which has the following occupation probabilities:

$$\left|20.445\text{ MeV}:\frac{3}{2}\frac{+}{2}\right\rangle = (0s)^{2.766}(0p)^{1.906}(sd)^{0.237}$$
$$\times(\text{other shells})^{0.091},$$
(11)

to be compared to the occupation probabilities for the ground state of ^{6}Li,

$$|^6\text{Li}:1_1^+\rangle = (0s)^{3.631}(0p)^{2.061}(sd)^{0.222}(\text{other shells})^{0.087}.$$
(12)

Note that the fact that the calculated energy of this $J^\pi=\frac{3}{2}^+$ state is about 3.7 MeV higher than experiment is more or less consistent with what we have seen in the case of ^{4}He where the "$1\hbar\Omega$" low-lying negative-parity states came out about 2–3 MeV higher than experiment. It will be interesting to track the energies of these states as well as the excited states in ^{4}He with increasing model-space size.

Above the two SP states (the ground $\frac{3}{2}_1^-$ state and the first excited $\frac{1}{2}_1^-$ state) and below the 20.445 MeV $\frac{3}{2}_2^+$ state, our calculation also gives three positive-parity "$1\hbar\Omega$" states, a $\frac{1}{2}^+$ state at 7.437 MeV and nearly de-

generate $\frac{5}{2}^+$ and $\frac{3}{2}^+$ states at 14.206 and 14.439 MeV, respectively. These states are dominated by the configurations $(0s)^4(sd)^1$ and $(0s)^3(0p)^2$. The occupancies of the orbitals in the model space are

$$\left| 7.437\text{MeV} : \frac{1}{2}\,_1^+ \right\rangle = (0s)^{3.219}(0p)^{0.933}(sd)^{0.681}$$
$$\times (\text{other shells})^{0.167}, \quad (13)$$

$$\left| 14.206\text{MeV} : \frac{5}{2}\,_1^+ \right\rangle = (0s)^{3.197}(0p)^{0.928}(sd)^{0.671}$$
$$\times (\text{other shells})^{0.204}, \quad (14)$$

$$\left| 14.439\text{MeV} : \frac{3}{2}\,_1^+ \right\rangle = (0s)^{3.153}(0p)^{1.011}(sd)^{0.623}$$
$$\times (\text{other shells})^{0.213}. \quad (15)$$

There have been previous theoretical predictions [34, 42] that there is a $\frac{1}{2}^+$ state at about 5 MeV and $\frac{3}{2}^+$ and $\frac{5}{2}^+$ states at about 12 MeV. These predictions have not been fully confirmed experimentally, but they are well supported by our results, again, keeping in mind that our calculated "$1\hbar\Omega$" states are probably about 2 or 3 MeV too high.

In addition to the above low-lying states, we have also listed in Table I a few other bound states of ^{5}He which have an energy not much higher than the experimental 16.75 MeV state.

The low-lying energy spectrum of ^{6}Li obtained in this calculation does not show much improvement over that in Ref. [16]. It again appears to be more spread out than the experimental spectrum.

C. $M1$ and $E2$ moments

Since we are using a large no-core model space, we choose to use bare operators ($e_p=1$, $e_n=0$, $g_p^s=5.586$, $g_n^s = -3.826$, $g_p^l=1.0$, $g_n^l=0.0$) to calculate the magnetic dipole ($M1$) and electric quadrupole ($E2$) moments in leading approximation. The calculated results are also given in Table I. It should be emphasized that only the nucleonic degrees of freedom are taken into account in calculating these moments. Proper considerations have to be given to the effects of the meson exchange currents (MEC's) before critical conclusions can be drawn from the comparison of the calculated moments (especially the $M1$ moment) with data.

The calculated $M1$ moment μ for the deuteron is $0.857\mu_N$. This agrees with the experimental result of $0.8574\mu_N$. However, this fortuitous agreement will be vitiated to the extent that the ignored MEC contribution is significant. Even if the MEC effect is negligible, the value that we obtained for the deuteron $M1$ moment is not theoretically exact. This is made evident in the discussion below.

The deuteron $M1$ moment is related to the D-state probability P_D as

$$\mu(^2\text{H}) = P_S \mu(^3S_1) + P_D \mu(^3D_1)$$
$$= (1 - P_D)0.880 + P_D 0.310 \; (\mu_N). \quad (16)$$

With this equation, a calculated value of $0.857\mu_N$ for $\mu(^2\text{H})$ leads to $P_D=4.0\%$. However, the exact P_D for the Reid93 potential is in fact 5.7% [43], implying a $\mu(^2\text{H})$ of $0.848\mu_N$. We, therefore, see that the tensor force is somehow weakened when we go from the bare NN potential to the effective shell-model interaction in Eq. (6) for our no-core model space. This infers the size of the neglected contribution to the magnetic moment operator arising in the theory of effective operators. It has been shown in Ref. [44] that the tensor force strength can be further reduced by core-polarization diagrams (mainly the Bertsch bubble diagram [45]) that one must take into account when calculating the effective interaction for a small, one-major-shell, model space outside an inert core.

The calculated deuteron quadrupole moment Q is $0.242e\,\text{fm}^2$, somewhat smaller than the experimental value of $0.286e\,\text{fm}^2$. This agrees with the above observation that the effective tensor force in our no-core shell-model interaction is weaker than that in the original NN potential. The reduced quadrupole moment may also arise from the fact that its operator involves a radial dependence (r^2) which needs to be renormalized when we truncate the infinite Hilbert space to our finite-size no-core HO model space. Thus we reason that, for our model space, the renormalization effects are larger for the $E2$ operator than for the $M1$ operator which does not have a radial dependence.

The need for using an effective operator to evaluate the root-mean-squared (rms) radius (or any other observable that involves it) is evident from Table I, where the calculated rms *point* radius $\sqrt{\langle r_p^2 \rangle}$ for the proton in the deuteron is 1.488 fm, significantly smaller than the experimental value of 1.95 fm. The large renormalization of the rms radius operator required for the deuteron is not surprising since it is a very loosely bound system; the wave function obtained in the truncated HO model space does not represent the exact wave function very well. The calculated $\sqrt{\langle r_p^2 \rangle}$ value for ^{6}Li is also smaller than the experimental value. However, the results of $\sqrt{\langle r_p^2 \rangle}$ for ^{3}H and ^{4}He are in good agreement with experiment. Note that we have evaluated these rms radii with "intrinsic" wave functions, and so the quoted results are free of spurious c.m. contributions.

Our calculated $M1$ moment for the triton is $2.659\mu_N$, about 11% smaller than the experimental value of $2.979\mu_N$. To a large extent, this discrepancy may be explained by the MEC effects that we have not taken into account. Indeed, in Ref. [40], it is shown that the inclusion of the MEC effects in a model-dependent way leads to a 14% increase in the triton $M1$ moment from $2.588\mu_N$ to $3.010\mu_N$, in close agreement with experiment.

For the ground state of ^{5}He, the calculated $M1$ and $E2$ moments are $-1.864\mu_N$ and $-0.332e\,\text{fm}^2$, respectively. Again, the MEC effects have to be considered when comparing these results with experimental data, which, to our knowledge, are not available.

It has been difficult in the past for theory to reproduce the $E2$ moment for the ground state of ^{6}Li. However, the calculated $E2$ moment is $-0.116e\,\text{fm}^2$, which is remark-

ably close to the experimental value of $-0.082e$ fm^2. Our calculated $M1$ moment is $0.851\mu_N$, which is about 3.5% higher than the experimental result of $0.822\mu_N$.

D. Effects of the Coulomb interaction

Since we include the Coulomb interaction, the isospin symmetry is not strictly conserved. But the isospin impurity caused by the Coulomb interaction is generally very small. For the bound states of ^{3}H and ^{3}He, the calculated values for isospin,

$$T_{\text{calc}} = \frac{\sqrt{4\langle\hat{T}^2\rangle + 1} - 1}{2}, \qquad (17)$$

are 0.500 000 and 0.500 022, respectively. Note that ^{3}H has only one proton, and so isospin is still a good quantum number. In ^{3}He, the calculated isospin shows only a 0.0044% deviation from the half-integer value. T_{calc} is 0.000 046 for the ground state of ^{4}He; it is 0.500 016 and 0.500 024 for the ground states of ^{5}He and ^{5}Li, respectively. The small isospin impurity for the ground states in these nuclei is due to the fact that all these states do not have any nearby state with the same J^π but a different T. From perturbation theory, one knows that the relatively weak Coulomb interaction will not induce much isospin mixing to these isolated states.

The Coulomb interaction has sizable effects on the absolute energies of the system, as is well known. Our calculation shows that, due to the Coulomb repulsion, the binding energy of ^{3}He is 0.725 MeV less than that of ^{3}H and the binding energy of ^{5}Li is 1.024 MeV less than that of ^{5}He. The experimentally observed differences in the binding energies for the above two pairs are 0.764 and 1.073 MeV, respectively. They are quite close to our calculated values, as one might expect since the Coulomb interaction is a perturbation in these light systems. Nevertheless, our results for the Coulomb energy are model dependent [in that the matrix elements of the Coulomb interaction in the shell-model Hamiltonian (6) were evaluated using a HO basis and possible renormalization corrections from the excluded space were ignored]. A smaller Coulomb effect of about 0.64 MeV was obtained in a more model-independent analysis [46] for the ^{3}H-^{3}He pair. It is also believed that other charge-symmetry-breaking effects contribute to the difference between the binding energies of ^{3}H and ^{3}He as well [47].

E. Dependence on $\hbar\Omega$ and Δ

The results presented so far are for the basis parameter $\hbar\Omega$ fixed at 14 MeV and the starting-energy parameter Δ fixed at -35 MeV. We will now discuss the sensitivity of the results on $\hbar\Omega$ and Δ. Table II shows calculated results for selected properties of ^{4}He for a few different choices of $\hbar\Omega$ and Δ. The degree of independence of the results on these two parameters is a measure of the convergence, which is related to the size of the model space.

We first fix Δ at -35 MeV and vary $\hbar\Omega$ from 14 MeV to 17 MeV and then to 20 MeV. The ground-state binding energy E_B of ^{4}He shows a variance of less than 2%; it increases from 28.757 MeV for $\hbar\Omega=14$ MeV to 28.879 MeV for $\hbar\Omega=17$ MeV and then decreases to 28.336 MeV for $\hbar\Omega=20$ MeV. A more stringent test of the convergence comes from the rms radius, which, in a $0\hbar\Omega$ HO shell-model calculation, would be proportional to $(\hbar\Omega)^{-1/2}$ and would, therefore, show some 16%'s decrease when $\hbar\Omega$ is increased from 14 MeV to 20 MeV. Our $6\hbar\Omega$ results for the proton rms point radius $\sqrt{\langle r_p^2\rangle}$ are 1.488 fm for $\hbar\Omega=14$ MeV, 1.434 fm for $\hbar\Omega=17$ MeV, and 1.428 fm for $\hbar\Omega=20$ MeV, showing a decrease of only 4%. In a zeroth-order estimate, the excitation energy $E_x(0_2^+,0)$ of the first excited 0^+ state is $2\hbar\Omega$. Our $6\hbar\Omega$ results are 26.135 MeV for $\hbar\Omega=14$ MeV, 25.934 MeV for $\hbar\Omega=17$ MeV, and 27.704 MeV for $\hbar\Omega=20$ MeV. These results show a rather weak dependence on the choice of $\hbar\Omega$. Note that the above results for $E_x(0_2^+,0)$ are still several MeV higher than experiment, but they can be further improved (i.e., lowered) within the same model space by employing an excitation-dependent effective interaction [20].

We then fix $\hbar\Omega$ at 14 MeV and vary Δ from -20 MeV to -35 MeV and to -50 MeV. The results are also shown in Table II. As one would expect, the ground-state binding energy E_B of ^{4}He decreases with decreasing Δ. As Δ decreases from -20 MeV to -50 MeV, E_B decreases by 19.7% from 32.864 MeV to 26.389 MeV. Again, these should be compared to the corresponding $0\hbar\Omega$ results, which are 35.805 MeV for $\Delta=-20$ MeV and 23.797 MeV for $\Delta=-50$ MeV, a change of 33.5%. The change in the rms radius is 4% when Δ decreases from -20 MeV to -50 MeV. Note that the rms radius anticorrelates with the binding energy: As we decrease Δ, the binding energy decreases while the rms radius increases.

It should be pointed out that for $\hbar\Omega=14$ MeV, the

TABLE II. Selected properties of ^{4}He in the $6\hbar\Omega$-space calculation for various values of the HO parameter $\hbar\Omega$ and the starting-energy parameter Δ. The results for $\hbar\Omega=14$ MeV and $\Delta=-35$ MeV from Table I are repeated here for the sake of comparison.

Observable	$\Delta = -35$ MeV			$\hbar\Omega = 14$ MeV		
	$\hbar\Omega=14$	$\hbar\Omega=17$	$\hbar\Omega=20$	$\Delta=-20$	$\Delta=-35$	$\Delta=-50$
E_B(MeV)	28.757	28.879	28.336	32.864	28.757	26.389
$\sqrt{\langle r_p^2\rangle}$(fm)	1.488	1.434	1.428	1.439	1.488	1.499
$E_x(0_2^+,0)$(MeV)	26.135	25.934	27.704	26.661	26.135	23.240

choice $\Delta=-50$ MeV, yielding a binding energy of 26.389 MeV, is probably more appropriate, since most realistic NN potentials are found to underbind ^{4}He by a few MeV (see, e.g., Ref. [38]). With $\Delta=-50$ MeV, the excitation energy $E_x(0_2^+,0)$ is 23.240 MeV, only 3 MeV above the experimental value.

IV. CONCLUSIONS

In this work, we have constructed an effective interaction for a six-major-shell no-core model space from a new, Reid-like, NN potential (known as Reid93) from the Nijmegen group [19]. The effective interaction has been applied to calculate nuclear structure properties for a few light nuclei, ranging from the deuteron to ^{6}Li. The results are very encouraging. Not only are the binding energies of these nuclei well reproduced, the energy spectra are also in good agreement with experiment. In particular, the experimental level sequence of the low-lying negative-parity states in ^{4}He is correctly reproduced, although the excitation energies are about 2–3 MeV higher than experiment. Based on our current and previous efforts, we expect that this discrepancy will be reduced as we more closely satisfy the dual convergence criteria, convergence against increasing N_{max} and d, where N_{max} signifies the highest unperturbed energy of the configurations taken into account and d represents the number of SP states included in the model space.

The magnetic dipole and electric quadrupole moments, calculated using bare operators with meson-exchange-current effects neglected, are also in reasonable agreement with experiment.

For ^{5}He, in addition to the two low-lying SP negative-parity states $\frac{3}{2}^-$ and $\frac{1}{2}^-$, we have obtained a low-lying $\frac{1}{2}^+$ state at about 7.4 MeV and two nearly degenerated states ($\frac{5}{2}^+$ and $\frac{3}{2}^+$) at 14.2 MeV and 14.4 MeV. The latter three, dominated by the configuration $(0s)^4(sd)^1$, are mainly SP states with one (sd) neutron coupled to

the ground state of ^{4}He. The actual energies of these predominantly "$1\hbar\Omega$" states could be about a few MeV lower, as in the case of ^{4}He. The previous theoretical predictions of a $\frac{1}{2}^+$ state at about 5 MeV and $\frac{5}{2}^+$ and $\frac{3}{2}^+$ states at about 12 MeV are therefore well supported by our results. The 16.75 MeV state, resulting from the ground state of ^{6}Li with a $(0s)$ proton removed, is reproduced at an energy of 20.445 MeV.

The Coulomb interaction, which is included in the calculations, accounts for the bulk part of the differences in the experimental binding energies of mirror pairs (^{3}H-^{3}He and ^{5}He-^{5}Li). We have also seen that the Coulomb interaction induces a very small amount of isospin impurity to the ground states of the light nuclei considered.

An extension of the current approach to heavier $0p$-shell nuclei will be straightforward. Our results for $A=2$–6 have given us optimism that our approach would be able to give a good description of neighboring nuclei as well. This is presently being investigated.

Of course, since the size of the shell-model matrix increases quite dramatically with an increasing number of nucleons, it is unlikely at the present time that one can apply the no-core approach to a much heavier nucleus, like ^{40}Ca. In this regard, the Monte Carlo shell-model approach [48], in which the size of the calculations increases only moderately with the number of active nucleons, offers some promise.

ACKNOWLEDGMENTS

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