

## Effects of the single-particle potential insertions in the effective interaction

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We investigate the effects of the single-particle potential insertions in the effective interaction by comparing energy spectra obtained from different treatments of these insertions as a function of the size of the no-core model space. The Brueckner reaction matrix used in the first calculation includes the single-particle potential insertions in ladder diagrams to all orders, while the Brueckner reaction matrix used in the second calculation only keeps the single-particle potential term in the lowest-order ladder diagram. The two calculations yield almost identical ground-state energies and low-lying excitation spectra for  ${}^4\text{He}$  and  ${}^6\text{Li}$  for *large enough* no-core model spaces, indicating that the effects of the single-particle potential insertions in second- and higher-order ladder diagrams are small. We explain the reason for the diminishing role of these insertions with increasing size of the model space. We also show that, through a standard method of instilling a single center-of-mass wave function into all low-lying states, the spurious center-of-mass kinetic-energy term shifts the energies of all the low-lying states by nearly a constant and, therefore, has little effect on the excitation spectrum.

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### I. INTRODUCTION

Since the investigations of Starkand and Kirson [1], it has generally been accepted that an order-by-order treatment of single-particle (SP) potential ( $U$ ) insertions is not an adequate procedure in developing an effective interaction. In their treatment, they took a fixed  $s$ - $d$  shell-model space and studied the effects on  $A=17$  and 18 nuclei as a function of the order in perturbation theory through which the  $U$  insertions were included. They showed that an order-by-order approach appeared to be slowly convergent and that putting the SP potential insertions in using perturbation theory could produce misleading results.

In this work we investigate two different treatments of the SP potential insertions. We compare the results for the low-lying energy spectra of  ${}^4\text{He}$  and  ${}^6\text{Li}$  obtained from two effective Hamiltonians, one of which is "exact," that is, we include the  $U$  term in ladder diagrams to all orders in calculating the  $G$  matrix; the other is approximate but conventional, for which the  $U$  term is kept only in the lowest-order ladder diagram (i.e., the diagram with only one interaction line). As the size of the model space increases, the differences in the two treatments of the  $U$  insertions decrease rapidly for reasons that we will make clear. Our conclusions are especially applicable to problems with few active nucleons, where large model spaces can be utilized.

In Sec. II, formalisms for the two methods are outlined. Section III discusses the calculation of the effective interaction, followed by Sec. IV, where the effects of the two methods on the low-lying spectra of  ${}^4\text{He}$  and  ${}^6\text{Li}$  are shown along with a discussion of the SP insertions and their role. Also, the effect of the spurious c.m.

component of the kinetic-energy operator on energy spectra is assessed, by comparing the above results for  ${}^4\text{He}$  and  ${}^6\text{Li}$  to calculations where the c.m. component of the kinetic-energy operator has been retained in the nuclear Hamiltonian.

### II. FORMALISM

The conventional nuclear Hamiltonian is written

$$H' = T + V = \sum_{i=1}^A t_i + \sum_{i<j}^A v_{ij} = H + T_{\text{c.m.}}, \quad (1)$$

where  $t_i$  is the one-body kinetic-energy operator and  $v_{ij}$  is the two-body  $NN$  potential. The Hamiltonian  $H'$  contains the spurious c.m. kinetic energy,  $T_{\text{c.m.}}$ , which is not present in the exact Hamiltonian  $H$ . In standard effective interaction calculations, a one-body SP potential,  $U$ , is added to and subtracted from  $H'$  to yield

$$\begin{aligned} H' &= \sum_{i=1}^A (t_i + u_i) + \left( \sum_{i<j}^A v_{ij} - \sum_{i=1}^A u_i \right) \\ &= (T + U) + (V - U) = H_0 + H_I, \end{aligned} \quad (2)$$

where eigenstates and eigenenergies of the unperturbed Hamiltonian,  $H_0$ ,

$$H_0 | \phi_{0i} \rangle = \epsilon_{0i} | \phi_{0i} \rangle \quad (3)$$

define the SP basis and the SP spectrum for the calculation. The residual interaction  $H_I = V - U$  is then used to calculate the Brueckner two-particle  $G$  matrix [2] (the two-particle ladder diagrams to all orders), which is the usual starting point for constructing the two-body effective

tive interaction for shell-model calculations.

In practical calculations for the  $G$  matrix, a harmonic-oscillator basis is often used. However, the  $U$  insertion is usually ignored in the calculation of the  $G$  matrix, leaving only  $H_I = V$  as the source of the effective interaction. The neglected  $U$  term is sometimes perturbatively inserted back into the diagrams for calculating the effective

interactions based on the Brueckner reaction matrix  $G$  [3, 4]. But, as noted in Ref. [1], such a perturbative treatment of the  $U$ -insertions is often ambiguous and incomplete.

In a harmonic-oscillator SP basis, the SP potential,  $U$ , for  $A$  particles can be written in terms of its relative and c.m. components:

$$U = \sum_{i=1}^A \frac{1}{2} m \Omega^2 \mathbf{r}_i^2 = \frac{2}{A} \sum_{i<j}^A \frac{1}{2} \frac{m}{2} \Omega^2 (\mathbf{r}_i - \mathbf{r}_j)^2 + \frac{mA}{2} \Omega^2 \left( \frac{\sum_{i=1}^A \mathbf{r}_i}{A} \right)^2 \equiv \frac{2}{A} \sum_{i<j}^A u_{ij} + \frac{mA}{2} \Omega^2 \mathbf{R}^2, \quad (4)$$

where we define  $\mathbf{R} = (\sum_{i=1}^A \mathbf{r}_i)/A$  and  $u_{ij} = \frac{1}{2} \frac{m}{2} \Omega^2 (\mathbf{r}_i - \mathbf{r}_j)^2$ . With the above equality we rewrite Eq. (2) as

$$H' = \sum_{i=1}^A h_i + \sum_{i<j}^A \left[ v_{ij} - \frac{2}{A} u_{ij} \right] - \frac{mA}{2} \Omega^2 \mathbf{R}^2 \equiv H_0 + \sum_{i<j}^A \tilde{v}_{ij} - U_{\text{c.m.}}, \quad (5)$$

where  $H_0 = \sum_{i=1}^A h_i$  with  $h_i = t_i + u_i$ ,  $U_{\text{c.m.}} = \frac{1}{2} (mA) \Omega^2 \mathbf{R}^2$ . We also define

$$\tilde{v}_{ij} = v_{ij} - \frac{2}{A} u_{ij}. \quad (6)$$

Similarly, the nonspurious (i.e., the c.m. kinetic energy removed) nuclear Hamiltonian  $H$  [see Eq. (1)] can be rewritten as

$$H = H' - T_{\text{c.m.}} = H_0 + \sum_{i<j}^A \tilde{v}_{ij} - H_{\text{c.m.}}. \quad (7)$$

The corresponding Brueckner two-particle  $G$  matrix [2] is given by

$$\begin{aligned} \tilde{G}_{12}(\omega) &= \tilde{v}_{12} + \tilde{v}_{12} \frac{Q_{2p}}{\omega - (h_1 + h_2 + \tilde{v}_{12})} \tilde{v}_{12} \\ &\equiv \tilde{G}'_{12}(\omega) - \frac{2}{A} u_{12}, \end{aligned} \quad (8)$$

where we for later convenience define

$$\tilde{G}'_{12}(\omega) = v_{12} + \tilde{v}_{12} \frac{Q_{2p}}{\omega - (h_1 + h_2 + \tilde{v}_{12})} \tilde{v}_{12}. \quad (9)$$

With a no-core model space [5, 6], the effective two-body interaction becomes particularly simple, containing only the Brueckner reaction matrix  $G$  plus the two-body folded-diagram series.

The starting energy,  $\omega$ , in the  $G$  matrix represents the energy of the two particles where they appear in a given process. In principle, this energy is well defined, but in practice, it is difficult to incorporate exactly, due to its dependence on spectator particles. Also, in principle, the calculation should be independent of the starting energy if the perturbation series for the effective interaction is computed to all orders, although in practice this is never done, except for special cases using the Lee-Suzuki iteration procedure [7]. Because  $G$  depends sensitively on  $\omega$ , i.e., the value of  $G$  tends to become more negative as  $\omega$  becomes more positive, we will treat  $\omega$  as a free parameter to optimize agreement with the experimental value for the binding energy. It has been shown that an op-

timal choice of the starting energy can minimize certain higher-order terms, such as the folded diagrams [8]. Our main justification for this approximate treatment of  $\omega$  is that, as the model space increases, the  $\omega$  dependence of the results decreases [5].

In this work, the effective interaction is taken to be the Brueckner reaction matrix evaluated at an empirically determined value of  $\omega$ . Therefore, our effective Hamiltonian is given by

$$\mathcal{H} = \sum_{i=1}^A h_i + \sum_{i<j}^A \tilde{G}_{ij} - H_{\text{c.m.}}. \quad (10)$$

Using the definition for  $\tilde{G}'_{ij}$  in Eq. (9), we can rewrite this effective Hamiltonian in a more transparent form ( $\mathcal{H} \equiv \mathcal{H}^{\text{ex}}$ ):

$$\mathcal{H}^{\text{ex}} = \left( \sum_{i=1}^A t_i - T_{\text{c.m.}} \right) + \sum_{i<j}^A \tilde{G}'_{ij} \equiv T_{\text{rel}} + \sum_{i<j}^A \tilde{G}'_{ij}, \quad (11)$$

which explicitly shows a relative kinetic-energy term (the usual one-body kinetic-energy term from which the c.m. component has been subtracted) as well as a “potential” term.

The results obtained for the above effective Hamiltonian,  $\mathcal{H}^{\text{ex}}$ , are referred to as “exact” results, and they are compared to the results obtained from the following effective Hamiltonian,  $\mathcal{H}^{\text{app}}$ :

$$\begin{aligned} \mathcal{H}^{\text{app}} &= \sum_{i=1}^A h_i + \sum_{i<j}^A G_{ij} - H_{\text{c.m.}} \\ &= \left( \sum_{i=1}^A t_i - T_{\text{c.m.}} \right) + \sum_{i<j}^A G'_{ij} \\ &= T_{\text{rel}} + \sum_{i<j}^A G'_{ij}, \end{aligned} \quad (12)$$

leaving a term linear in the relative kinetic-energy opera-

tor plus the Brueckner reaction matrix, calculated without taking into account the higher-order  $U$  insertions. The reaction matrices,  $G_{12}$  and  $G'_{12}$ , are defined by

$$G_{12}(\omega) = v_{12} - \frac{2}{A}u_{12} + v_{12} \frac{Q_{2p}}{\omega - (h_1 + h_2 + v_{12})}v_{12} \\ \equiv G'_{12}(\omega) - \frac{2}{A}u_{12}, \quad (13)$$

$$G'_{12}(\omega) = v_{12} + v_{12} \frac{Q_{2p}}{\omega - (h_1 + h_2 + v_{12})}v_{12}. \quad (14)$$

Note that  $G'_{12}$  differs from  $\tilde{G}'_{12}$  in Eq. (9) [or  $G_{12}$  from  $\tilde{G}_{12}$  in Eq. (8)] in that the two-body  $U$  insertion ( $-\frac{2}{A}u_{ij}$ ) is neglected in the second term in Eq. (14) [or Eq. (13)], which corresponds to ladder diagrams with two or more interaction ( $V$ ) lines. The resulting effective Hamiltonian,  $\mathcal{H}^{\text{app}}$ , is, therefore, not exact. It should be pointed out that this approximate  $G$  matrix  $G'_{ij}$  has often been used in the past to obtain effective interactions in calculations for which all higher-order  $U$  insertions are systematically neglected.

### III. SHELL-MODEL RESULTS

For the free  $NN$  interaction we use the Reid soft-core potential [9] as modified for the inclusion of higher-partial waves by Day [10]. To both the effective Hamiltonians in Eqs. (11) and (12)  $\lambda(H_{\text{c.m.}} - \frac{3}{2}\hbar\Omega)$  with  $\lambda \gg 1$  is added to ensure that the c.m. motion for all low-lying states of the spectra is in its lowest c.m. configuration. The shell-model diagonalization is carried out with the OXBASH shell-model code [11]. Calculations for  ${}^4\text{He}$  are performed employing no-core model spaces starting with the  $0s$  shell successively adding one shell at a time until the  $1p0f$  shell is included. These model spaces are referred to as the  $N=1$ ,  $N=2$ ,  $N=3$ , and  $N=4$  spaces, respectively. No restrictions are imposed on the shell-model diagonalizations in those model spaces. Table I displays the results for the two Hamiltonians in the four different model spaces for  ${}^4\text{He}$ , employing a starting energy of  $\omega = 7$  MeV and an oscillator parameter of  $\hbar\Omega = 21$  MeV. The third column displays results calculated with a nuclear Hamiltonian in which the spurious c.m. component of the kinetic-energy operator  $T_{\text{c.m.}}$  has been retained. This is discussed further below. The last

TABLE I. The calculated ground-state energies and excitation energies of low-lying states of  ${}^4\text{He}$ , in units of MeV. The effective Hamiltonians  $\mathcal{H}^{\text{ex}}$ ,  $\mathcal{H}^{\text{app}}$ , and  $\mathcal{H}_t^{\text{app}}$  used in the calculations are defined in Eqs.(11), (12), and (15), respectively. The starting energy  $\omega = 7$  MeV and the oscillator parameter  $\hbar\Omega = 21$  MeV are chosen so as to yield a reasonable ground-state energy. The calculations are performed using the OXBASH shell-model program [11], in a no-core model space of different sizes, signified by  $N$ , the number of major shells contained. The experimental data are taken from Ref. [12] for  ${}^4\text{He}$ . The numbers in parentheses are taken from Ref. [13].

${}^4\text{He}$	$J^\pi$	$T$	$\mathcal{H}^{\text{ex}}$	$\mathcal{H}^{\text{app}}$	$\mathcal{H}_t^{\text{app}}$	Experiment
$N = 1$	$0_1^+$	0	-23.490	-26.128	-10.378	-28.296
$N = 2$	$0_1^+$	0	-24.087	-25.249	-9.735	-28.296
	$0_2^+$	0	57.152	60.357	60.607	20.21 (20.1)
	$0_1^-$	0	30.403	32.302	32.271	21.01 (21.1)
	$2_1^-$	0	31.406	32.932	33.053	21.84 (22.1)
	$2_1^-$	1	32.159	33.401	33.517	23.33 (26.4)
	$1_1^-$	1	35.546	37.401	37.440	23.64 (27.5)
	$1_1^-$	0	39.273	42.425	42.644	24.25 (31.0)
	$0_1^-$	1	35.278	37.566	37.834	25.28 (29.5)
	$1_2^-$	1	39.298	42.083	43.003	25.95 (30.5)
$N = 3$	$0_1^+$	0	-21.691	-21.386	-5.866	
	$0_2^+$	0	34.478	35.677	35.687	
	$0_1^-$	0	26.742	26.586	26.844	
	$2_1^-$	0	28.282	28.196	28.388	
	$2_1^-$	1	29.685	29.638	29.818	<sup>a</sup>
	$1_1^-$	1	33.084	33.079	33.314	
	$1_1^-$	0	35.943	36.205	36.510	
	$0_1^-$	1	32.276	32.351	32.581	
	$1_2^-$	1	37.697	37.079	38.300	
$N = 4$	$0_1^+$	0	-21.918	-21.955	-6.392	
	$0_2^+$	0	33.807	34.257	34.580	
	$0_1^-$	0	22.351	22.505	22.500	
	$2_1^-$	0	25.467	25.721	25.728	
	$2_1^-$	1	27.236	27.554	27.554	<sup>a</sup>
	$1_1^-$	1	27.545	27.791	27.861	
	$1_1^-$	0	30.443	30.804	30.827	
	$0_1^-$	1	29.137	29.491	29.493	
	$1_2^-$	1	29.741	30.063	30.050	

<sup>a</sup> See above.

column displays experimental values [12–14] for comparison. The results for the Hamiltonians in Eqs. (11) and (12) for all the model spaces improve in agreement as the size of the model space is increased. There is excellent agreement between the two Hamiltonians for the largest model space used, i.e.,  $N = 4$ . The ground-state energies differ by a few MeV for the  $N=1$  space and only by a few tens of keV for the  $N=4$  space calculations. In all calculations, the excited-state spectra display the same level systematics.

In the  ${}^6\text{Li}$  calculation, model spaces from  $N=2$  through  $N=4$  are employed. The  $N=2$  space calculation is performed without any many-body excitation restrictions. Excitations up to  $6\hbar\Omega$  are allowed for the  $N=3$  space calculation, and for the  $N=4$  space excitations up to  $4\hbar\Omega$  are allowed. These calculations are done for a starting energy of 20 MeV and an oscillator parameter of 16 MeV. In Table II, where the results for  ${}^6\text{Li}$  are displayed, the columns are arranged in the same manner as the columns in Table I. We see similar trends to those discussed for  ${}^4\text{He}$ . Because of the larger nuclear radius, the strength of the oscillator potential is decreased. Excellent agreement for the two Hamiltonians is seen already for the  $N=3$  space ground-state energies. The level systematics of the two approaches are in excellent agreement and the excitation spectra are within a few tens of keV for the largest space. The results for the two nuclei indicate that the two Hamiltonians are practically equivalent if

we employ large enough model spaces.

The origin of the trends we present is easy to find. We are examining the role of  $u_{12}$  in the higher-order terms of the  $G$  matrix. Note that  $u_{12}$  in these terms connects model space states with those in the  $Q = 1$  space and connects  $Q = 1$  space states with themselves. As the  $Q = 0$  space expands, there are fewer  $U$  interactions. For two-particle states within the model space, the cancellation of  $U$  insertions is exact in both treatments. Thus, for two-particle states within the model space, the only reflection of the choice of  $U$  is in the basis-state wave functions which are the same in both of our calculations. Furthermore, the harmonic-oscillator potential,  $u_{12}$ , connects only two-particle states differing by at most  $2\hbar\Omega$ , so that the states it affects most are at the boundary between the  $Q$ -space and the  $P$ -space states. As the size of the model space,  $P$ , increases, this boundary recedes from the states which have the greatest influence on the low-lying spectra.

In Tables I and II we also display the results for an effective Hamiltonian which retains the c.m. kinetic-energy term:

$$\mathcal{H}_t^{\text{app}} = \sum_{i=1}^A t_i + \sum_{i<j}^A G'_{ij} = \mathcal{H}^{\text{app}} + T_{\text{CM}}. \quad (15)$$

Again,  $\lambda(H_{\text{c.m.}} - \frac{3}{2}\hbar\Omega)$  is added to the above Hamiltonian in the shell-model calculations. The results for this

TABLE II. The calculated ground-state energies and excitation energies of low-lying states of  ${}^6\text{Li}$ , in units of MeV. The effective Hamiltonians  $\mathcal{H}^{\text{ex}}$ ,  $\mathcal{H}^{\text{app}}$ , and  $\mathcal{H}_t^{\text{app}}$  used in the calculations are defined in Eqs. (11), (12), and (15), respectively. The starting energy  $\omega = 20$  MeV and the oscillator parameter  $\hbar\Omega = 16$  MeV are chosen so as to yield a reasonable ground-state energy. The calculations are performed using the OXBASH shell-model program [11], in a no-core model space of different sizes, signified by  $N$ , the number of major shells contained. Unless indicated, there is no restriction imposed on nucleon configurations within the model space. The experimental data are taken from Ref. [14]. When significant (and available), the error bars are given for the experimental results.

${}^6\text{Li}$	$J^\pi$	$T$	$\mathcal{H}^{\text{ex}}$	$\mathcal{H}^{\text{app}}$	$\mathcal{H}_t^{\text{app}}$	Experiment
$N = 2$	$1_1^+$	0	-28.020	-30.200	-18.375	-31.996
	$3_1^+$	0	2.165	1.657	1.689	2.186
	$0_1^+$	1	3.036	3.097	3.142	3.563
	$2_1^+$	0	3.810	3.920	3.966	$4.31 \pm 0.022$
	$2_1^+$	1	5.080	5.047	5.092	$5.366 \pm 0.015$
	$1_2^+$	0	7.059	7.339	7.368	$5.65 \pm 0.05$
$N = 3^{\text{a}}$	$1_1^+$	0	-28.296	-28.814	-16.881	
	$3_1^+$	0	3.307	3.231	3.224	
	$0_1^+$	1	3.079	3.038	3.048	
	$2_1^+$	0	5.991	6.123	6.115	<sup>c</sup>
	$2_1^+$	1	6.295	6.249	6.253	
	$1_2^+$	0	8.166	8.263	8.279	
$N = 4^{\text{b}}$	$1_1^+$	0	-25.477	-25.300	-13.373	
	$3_1^+$	0	3.078	3.077	3.075	
	$0_1^+$	1	3.313	3.311	3.305	
	$2_1^+$	0	4.880	4.866	4.867	<sup>c</sup>
	$2_1^+$	1	6.210	6.214	6.211	
	$1_2^+$	0	7.023	7.260	7.260	

<sup>a</sup> In the  $N=3$  calculation, up to  $6\hbar\Omega$  excitations are allowed.

<sup>b</sup> In the  $N=4$  calculation, up to  $4\hbar\Omega$  excitations are allowed.

<sup>c</sup> See above.

effective Hamiltonian are compared to those of  $\mathcal{H}^{\text{ex}}$  of Eq. (11) and  $\mathcal{H}^{\text{app}}$  of Eq. (12). From the tables, it is clear that the inclusion of  $T_{\text{c.m.}}$  in a shell-model calculation appears only to shift the entire spectrum by nearly a constant and does not affect the excitation-energy spectrum. This constant is largely governed by the virial theorem and is about  $\frac{1}{2}(\frac{3}{2}\hbar\Omega)$ : 15.75 MeV for  ${}^4\text{He}$  and 12 MeV for  ${}^6\text{Li}$ . This is not surprising, because we force the c.m. motion to be in its lowest c.m. configuration by adding  $\lambda(H_{\text{c.m.}} - \frac{3}{2}\hbar\Omega)$  to the Hamiltonians. In fact, the degree to which the shift is a constant is a measure of the degree to which each state has the same c.m. wave function. The trend of our calculation indicates that the elimination of the spurious c.m. wave functions generally improves with the increasing of the size of the model space.

#### IV. CONCLUSION

Two effective Hamiltonians have been used to calculate the low-lying energy spectra for  ${}^4\text{He}$  and  ${}^6\text{Li}$  in various no-core model spaces. The first effective Hamiltonian is obtained from the Brueckner reaction matrix which includes the SP potential insertions in the ladder diagrams to all orders. The second effective Hamiltonian is obtained from the reaction matrix which only keeps the SP potential term in its lowest order, i.e., the higher-order insertions are neglected from the ladder diagrams with two or more interaction lines. Shell-model results for these two effective Hamiltonians are in remarkable agreement with each other for both nuclei under consideration, especially when large no-core model spaces are employed. The results indicate that the higher-order SP potential insertions have a negligible effect on low-

lying nuclear-energy spectra, when the above outlined prescription is used as a starting point for constructing effective shell-model Hamiltonians. Furthermore, including the c.m. kinetic-energy term  $T_{\text{c.m.}}$  in the nuclear Hamiltonian merely shifts the whole energy spectrum up by an amount  $\frac{1}{2}(\frac{3}{2}\hbar\Omega)$ ; hence, it can be ignored in a calculation for the excitation spectrum, or replaced by a constant  $\frac{1}{2}(\frac{3}{2}\hbar\Omega)$ , provided that spurious c.m. excitations are eliminated from the low-lying spectrum by the addition of  $\lambda(H_{\text{c.m.}} - \frac{3}{2}\hbar\Omega)$  ( $\lambda \gg 1$ ) in the shell-model diagonalization.

It is found that the convenient choice of  $T_{\text{rel}} + G$  for the effective shell-model Hamiltonian yields accurate results in the large ( $N = 4$ ) model space. This choice greatly simplifies calculations, because  $G$  is calculated using only  $v_{ij}$  and, hence, is  $A$  independent. Thus,  $G$  can be calculated and stored and used for calculating the structure of several neighboring nuclei.

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