No-core shell-model calculations with starting-energy-independent multivalued effective interactions

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Large-space no-core shell-model calculations have been performed for ^{3}H, ^{4}He, ^{5}He, ^{6}Li, and ^{6}He, using a starting-energy-independent two-body effective interaction derived by application of the Lee-Suzuki similarity transformation. This transformation can be performed by direct calculation or by different iteration procedures, which are described. A possible way of reducing the auxiliary potential influence on the two-body effective interaction has also been introduced. The many-body effects have been partially taken into account by employing the recently introduced multivalued effective interaction approach. Dependence of the ^{5}He energy levels on the harmonic-oscillator frequency as well as on the size of the model space has been studied. The Reid 93 nucleon-nucleon potential has been used in the study, but results have also been obtained using the Nijmegen II potential for comparison. [S0556-2813(96)03612-6]

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I. INTRODUCTION

Large-basis no-core shell-model calculations have recently been performed [1–8]. In these calculations all nucleons are active, which simplifies the effective interaction as no-hole states are present. In the approach taken, the effective interaction is determined for a system of two nucleons only and subsequently used in many-particle calculations. To take into account a part of the many-body effects a multivalued effective interaction approach was introduced and applied in the no-core shell-model calculations [8] and also tested in a model calculation [9].

In these shell-model calculations different approaches have been taken in deriving the two-nucleon effective interaction. All the methods employed, however, relied on the reference G-matrix method, introduced in Ref. [10], which leads to two-body matrix elements of a starting-energy-dependent G matrix. To get rid of this unwanted dependence either a suitable parametrization was chosen [4–6,8] or folded diagram effects were taken into account by calculating the derivatives of the G matrix in an approximate way [4,7].

In the present paper we apply the Lee-Suzuki similarity-transformation approach [11] to derive the two-body effective interaction. We try to avoid unnecessary approximations in performing the calculations. The harmonic-oscillator insertions are kept; consequently, the effective interaction is A dependent. Also the Hermitization of the effective interaction, which is, in general, non-Hermitian, is done without approximations by a similarity transformation.

We consider three possible ways of deriving the effective interaction. The first two are the standard iterative procedures, starting with the G-matrix calculation [10]. We study the Lee-Suzuki vertex renormalization iteration, which makes use of the G-matrix derivatives. Unlike most of the previous applications of this approach, we calculate these derivatives exactly employing the reference G-matrix derivatives. The other iterative procedure, usually referred to as the Krenciglowa-Kuo technique, is carried out by diagonalizing the non-Hermitian effective Hamiltonian in subsequent iterations [12]. This method has so far been applied only to model calculations. We also discuss its recent generalization [13]. Finally, we directly construct the effective interaction without calculating the G matrix by employing the solutions of the two-body problem. When criteria necessary for convergence are the same for both iteration procedures, the resulting effective interactions obtained in all three methods are identical. The last method, however, has two advantages: first, its simplicity and, second, the fact that it utilizes an explicit construction of the transformation operator. This transformation operator may then be used for the calculation of other effective operators.

To take partially into account the many-body effects neglected when using only a two-body effective interaction, we employ the recently introduced multivalued effective interaction approach [8].

It was observed earlier [7] that the two-body effective interaction derived by the vertex renormalization method is too attractive and leads to overbinding of the many-body system. We discuss this problem and believe that it is largely due to the uncompensated Q-space part of the auxilliary harmonic-oscillator potential. We discuss possible treatment of this problem by modification of that part of the auxilliary potential.

In Sec. II we discuss the shell-model Hamiltonian with a bound center of mass as well as the two-particle Hamiltonian and the methods used to derive the starting-energy-independent effective interaction. Results of the calculations for ^{3}H, ^{4}He, ^{5}He, ^{6}Li, and ^{6}He are presented in Sec. III. In particular, we discuss the harmonic-oscillator frequency and the model-space-size dependences of the ^{5}He states. Conclusions are given in Sec. IV.

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II. SHELL-MODEL HAMILTONIAN AND STARTING-ENERGY-INDEPENDENT EFFECTIVE INTERACTION

In most shell-model studies the one- and two-body Hamiltonian for the A-nucleon system, i.e.,

$$H=\sum_{i=1}^{A}\frac{\vec{p}_i^{\,2}}{2m}+\sum_{i<j}^{A}V_{ij}, \tag{1}$$

where m is the nucleon mass and V_{ij} the nucleon-nucleon interaction, is modified by adding the center-of-mass harmonic oscillator potential $\frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{R}=(1/A)\Sigma_{i=1}^{A}\vec{r}_i$. This potential does not influence intrinsic properties of the many-body system. It provides, however, a mean field ''felt'' by each nucleon and allows us to work with a convenient harmonic-oscillator basis. For an alternative manipulation of the center-of-mass terms, see, e.g., Ref. [1]. The modified Hamiltonian, depending on the harmonic-oscillator frequency Ω, can be written as

$$H^{\Omega}=\sum_{i=1}^{A}\left[\frac{\vec{p}_i^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right]+\sum_{i<j}^{A}\left[V_{ij}-\frac{m\Omega^2}{2A}(\vec{r}_i-\vec{r}_j)^2\right], \tag{2}$$

which is the same as Eq. (4) in Ref. [1]. Shell-model calculations are carried out in a model space defined by a projector P. In the present work we will always use a complete $N\hbar\Omega$ model space. The complementary space to the model space is defined by the projector $Q=1-P$. Consequently, for the P-space part of the shell-model Hamiltonian we get

$$H_P^{\Omega}=\sum_{i=1}^{A}P\left[\frac{\vec{p}_i^{\,2}}{2m}+\frac{1}{2}m\Omega^2\vec{r}_i^{\,2}\right]P+\sum_{i<j}^{A}P\left[V_{ij}-\frac{m\Omega^2}{2A}(\vec{r}_i-\vec{r}_j)^2\right]_{\rm eff}P. \tag{3}$$

The effective interaction appearing in Eq. (3) is, in general, an A-body interaction, and, if it is determined without any approximations, the model-space Hamiltonian provides an identical description of a subset of states as the full-space Hamiltonian (2). The intrinsic properties of the many-body system still do not depend on Ω. From among the eigenstates of the Hamiltonian (3), it is necessary to choose only those corresponding to the same center-of-mass energy. This can be achieved by projecting the center-of-mass eigenstates with energies greater than $\frac{3}{2}\hbar\Omega$ upwards in the energy spectrum. The shell-model Hamiltonian, which does this, takes the form

$$H_{P\beta}^{\Omega}=\sum_{i<j=1}^{A}P\left[\frac{(\vec{p}_i-\vec{p}_j)^2}{2Am}+\frac{m\Omega^2}{2A}(\vec{r}_i-\vec{r}_j)^2\right]P+\sum_{i<j}^{A}P\left[V_{ij}-\frac{m\Omega^2}{2A}(\vec{r}_i-\vec{r}_j)^2\right]_{\rm eff}P+\beta P(H_{\rm c.m.}^{\Omega}-\tfrac{3}{2}\hbar\Omega)P, \tag{4}$$

where β is a sufficiently large positive parameter and $H_{\rm c.m.}^{\Omega}=\vec{P}_{\rm c.m.}^{\,2}/2Am+\frac{1}{2}Am\Omega^2\vec{R}^2$, $\vec{P}_{\rm c.m.}=\Sigma_{i=1}^{A}\vec{p}_i$. In a complete $N\hbar\Omega$ model space the removal of the spurious center-of-mass motion is exact. When going from Eq. (3) to (4), we added $(\beta-1)PH_{\rm c.m.}^{\Omega}P$ and subtracted $\beta\frac{3}{2}\hbar\Omega P$, which has no effect on the intrinsic spectrum of states with the lowest center-of-mass configuration.

The effective interaction should be determined from H^{Ω} (2). Calculation of the exact A-body effective interaction is, however, as difficult as finding the full-space solution. Usually, the effective interaction is approximated by a two-body effective interaction determined from a two-nucleon problem. The relevant two-nucleon Hamiltonian obtained from Eq. (2) is then

$$H_2^{\Omega}\equiv H_{02}^{\Omega}+V_2^{\Omega}=\frac{\vec{p}_1^{\,2}+\vec{p}_2^{\,2}}{2m}+\frac{1}{2}m\Omega^2(\vec{r}_1^{\,2}+\vec{r}_2^{\,2})+V(\vec{r}_1-\vec{r}_2)-\frac{m\Omega^2}{2A}(\vec{r}_1-\vec{r}_2)^2. \tag{5}$$

This can be transformed into two-nucleon relative and center-of-mass parts by introducing the coordinates $\vec{q}=\frac{1}{2}(\vec{p}_1-\vec{p}_2)$, $\vec{P}_{\rm 2c.m.}=\vec{p}_1+\vec{p}_2$, $\vec{R}_{\rm 2c.m.}=\frac{1}{2}(\vec{r}_1+\vec{r}_2)$, and $\vec{r}=\vec{r}_1-\vec{r}_2$, yielding

$$H_2^{\Omega}=\frac{\vec{P}_{\rm 2c.m.}^{\,2}}{2M}+\frac{1}{2}M\Omega^2\vec{R}_{\rm 2c.m.}^{\,2}+\frac{\vec{q}^{\,2}}{2\mu}+\frac{A-2}{2A}\mu\Omega^2\vec{r}^{\,2}+V(\vec{r}), \tag{6}$$

with $M=2m$ and $\mu=\frac{1}{2}m$. While the center-of-mass part has the solution $E_{\mathcal{NL}}=(2\mathcal{N}+\mathcal{L}+\frac{3}{2})\hbar\Omega$ and the eigenvectors $|\mathcal{NL}\rangle$, the relative-coordinate part can be solved as a differential equation or, alternatively, can be diagonalized in a sufficiently large harmonic-oscillator basis. The latter possibility is, obviously, not applicable for hard-core potentials.

The starting-energy-dependent effective interaction or G matrix corresponding to a two-nucleon model space defined by the projector P_2 can be written as

$$G(\varepsilon)=V_2^{\Omega}+V_2^{\Omega}Q_2\frac{1}{\varepsilon-Q_2H_2^{\Omega}Q_2}Q_2V_2^{\Omega}, \tag{7}$$

where $Q_2=1-P_2$ and V_2^{Ω} is the interaction given by the last two terms on the right-hand side (RHS) of Eq. (5). The G matrix (7) can be constructed from the solutions of the Schrödinger equation with the Hamiltonian (5), by using the reference matrix method [10]. The G matrix can be expressed as

$$G(\varepsilon)=A(\varepsilon)^{-1}G_{\rm R}(\varepsilon), \tag{8a}$$

$$G_{\rm R}(\varepsilon)=(H_{02}^{\Omega}-\varepsilon)+(H_{02}^{\Omega}-\varepsilon)\sum_k\frac{|k\rangle\langle k|}{\varepsilon-E_k}(H_{02}^{\Omega}-\varepsilon), \tag{8b}$$

$$A(\varepsilon)=1+G_{\rm R}(\varepsilon)P_2\frac{1}{\varepsilon-H_{02}^{\Omega}}, \tag{8c}$$

where H_{02}^{Ω} is given by the first two terms on the RHS of Eq. (5) and E_k and $|k\rangle$ are the eigenvalues and eigenvectors of H_2^{Ω}, Eq. (5), respectively.

To obtain a starting-energy-independent effective interaction, one has to take into account the folded diagrams or, equivalently, to construct a similarity transformation that

guarantees decoupling between the model space P and the Q space. We employ the Lee-Suzuki [11] similarity transformation method, which gives the effective interaction in the form

$$P_2 V_{2\text{eff}} P_2 = P_2 V_2^{\Omega} P_2 + P_2 V_2^{\Omega} Q_2 \omega P_2 , \tag{9}$$

with ω satisfying the equations $\omega = Q_2 \omega P_2$ and

$$\omega = Q_2 \frac{1}{\varepsilon - Q_2 H_2^{\Omega} Q_2} Q_2 V_2^{\Omega} P_2 - Q_2 \frac{1}{\varepsilon - Q_2 H_2^{\Omega} Q_2} Q_2 \omega P_2 (H_2^{\Omega} + H_2^{\Omega} Q_2 \omega - \varepsilon) P_2 . \tag{10}$$

In this degenerate-model-space formulation two iterative solutions of Eq. (10) exist and lead to different expressions for the effective interaction. The first one, the Krenciglowa-Kuo (KK) iteration procedure [12], gives for the nth iteration formula

$$V_{2\text{eff},n} = \sum_l P_2 G(\varepsilon + E_{l,n-1}) P_2 |l_{n-1}\rangle \langle \tilde{l}_{n-1}| P_2 . \tag{11}$$

In Eq. (11) the states $|l_{n-1}\rangle$ are the right eigenvectors of $H_{02}^{\Omega} + V_{2\text{eff},n-1} - \varepsilon$ belonging to the eigenvalue $E_{l,n-1}$. The tilde states are the biorthogonal eigenvectors. When this procedure converges, it does so to the states which have the largest overlap with the model-space states. The resulting $V_{2\text{eff}}$ Eq. (9), is independent of the starting energy ε. This method was recently generalized to a nondegenerate model space [13]. The difference is in the starting iteration. When using Eq. (11), the starting iteration is $G(\varepsilon)$, while the nondegenerate model-space version [13] starts with

$$\sum_{\alpha} G(\varepsilon_{\alpha} + \Delta) P_{2\alpha} . \tag{12}$$

Here the ε_{α} are the unperturbed energies, in our case the two-nucleon harmonic-oscillator energies, and $P_{2\alpha}$ is the projector on the two-nucleon state $|\alpha\rangle$. Unlike in the original paper [13], we introduce a shift Δ, as the G matrix cannot be evaluated for the energy ε_{α}, using the reference matrix method (8). Note that Eq. (12) is the interaction used in the previous no-core shell-model studies [4–6,8] with Δ treated as a free parameter.

One can also use the alternative procedure, usually called the vertex-renormalization approach, which can be obtained from Eq. (10) [11]. The resulting iteration sequence for the effective interaction can be written as

$$H_{02}^{\Omega} + V_{2\text{eff},n} - \varepsilon = \left[P_2 - P_2 G^{(1)}(\varepsilon) P_2 - \sum_{m=2}^{n-1} \frac{1}{m!} P_2 G^{(m)}(\varepsilon) P_2 (H_{02}^{\Omega} + V_{2\text{eff},n-m+1} - \varepsilon) P_2 (H_{02}^{\Omega} + V_{2\text{eff},n-m+2} - \varepsilon) \times P_2 \cdots (H_{02}^{\Omega} + V_{2\text{eff},n-1} - \varepsilon) P_2 \right]^{-1} P_2 [H_{02}^{\Omega} + G(\varepsilon) - \varepsilon] P_2 , \tag{13}$$

where $V_{2\text{eff},1} = P_2 G(\varepsilon) P_2$. This method, which relies on the G matrix derivatives $G^{(m)}$, was applied in shell-model calculations for the first time by Poppelier and Brussard [14]. In that and most other applications different numerical approximations were used to evaluate the derivatives [4,7,14]. In fact, these derivatives can be calculated exactly, because the reference matrix $G_{\text{R}}(\varepsilon)$, Eq. (8b), as well as the operator $A(\varepsilon)$, Eq. (8c), can be differentiated to any order analytically, as can be seen when they are expressed in the two-nucleon harmonic-oscillator basis. For example, the nth derivative, $n>0$, of G_{R} is

$$G_{\text{R}\alpha\gamma}^{(n)}(\varepsilon) = (-1)^n n! \left[\sum_k \frac{\langle \alpha|k\rangle\langle k|\gamma\rangle}{(\varepsilon - E_k)^{n-1}} - (2\varepsilon - \varepsilon_{\alpha} - \varepsilon_{\gamma}) \times \sum_k \frac{\langle \alpha|k\rangle\langle k|\gamma\rangle}{(\varepsilon - E_k)^{n}} + (\varepsilon - \varepsilon_{\alpha}) \times \sum_k \frac{\langle \alpha|k\rangle\langle k|\gamma\rangle}{(\varepsilon - E_k)^{n+1}} (\varepsilon - \varepsilon_{\gamma}) \right], \tag{14}$$

and similarly for $A(\varepsilon)$. Then the nth G-matrix derivative can be expressed as

$$G^{(n)} = \sum_{m=0}^{n} \frac{n!}{(n-m)!\,m!} (A^{-1})^{(n-m)} G_{\text{R}}^{(m)} , \tag{15}$$

where the derivatives of the inverse matrix can be obtained from

$$(A^{-1})^{(n)} = -\sum_{m=0}^{n-1} \frac{n!}{(n-m)!\,m!} A^{-1} A^{(n-m)} (A^{-1})^{(m)} . \tag{16}$$

An alternative way of calculating G-matrix derivatives analytically was proposed in Ref. [15]. When the convergence of Eq. (13) is achieved, the effective interaction does not depend on the starting energy ε. The states reproduced in the model space are those lying closest to ε.

As our calculations start with exact solutions of the Hamiltonian (5), we are, in fact, in a position to construct the operator ω and, hence, the effective interaction directly from these solutions. Let us denote the two-nucleon harmonic-oscillator states, which form the model space, as $|\alpha_P\rangle$, and those which belong to the Q space, as $|\alpha_Q\rangle$. Then the Q-space components of the eigenvector $|k\rangle$ of the Hamil-

tonian (5) can be expressed as a combination of the P-space components with the help of the operator ω:

$$\langle \alpha_Q|k\rangle = \sum_{\alpha_P} \langle \alpha_Q|\omega|\alpha_P\rangle\langle \alpha_P|k\rangle. \tag{17}$$

If the dimension of the model space is d_P, we may choose a set $\mathcal{K}$ of d_P eigenevectors, for which the relation (17) will be satisfied. Under the condition that the $d_P \times d_P$ matrix $\langle \alpha_P|k\rangle$ for $|k\rangle \in \mathcal{K}$ is invertible, the operator ω can be determined from Eq. (17). Note that in the present application the eigenvectors $|k\rangle$ are direct products of the center-of-mass and the relative-coordinate eigenvectors. The condition of invertibility is not satisfied for an arbitrary choice of the eigenvector set $\mathcal{K}$. Once the operator ω is determined the effective Hamiltonian can be constructed as follows from Eq. (9):

$$\langle \gamma_P|H_{2\text{eff}}|\alpha_P\rangle = \sum_{k\in\mathcal{K}} \Bigg[\langle \gamma_P|k\rangle E_k \langle k|\alpha_P\rangle + \sum_{\alpha_Q} \langle \gamma_P|k\rangle E_k \langle k|\alpha_Q\rangle\langle \alpha_Q|\omega|\alpha_P\rangle \Bigg]. \tag{18}$$

It should be noted that $P_2|k\rangle = \Sigma_{\alpha_P}|\alpha_P\rangle\langle \alpha_P|k\rangle$ for $|k\rangle \in \mathcal{K}$ is a right eigenvector of Eq. (18) with the eigenvalue E_k.

In the case when the iteration conditions are the same for both methods (11) and (13), and the set $\mathcal{K}$, for which Eq. (17) is fulfilled, is chosen accordingly, all three methods lead to the identical effective Hamiltonian. This Hamiltonian, when diagonalized in a model-space basis, reproduces exactly the set $\mathcal{K}$ of d_P eigenvalues E_k. Note that the effective Hamiltonian is, in general, non-Hermitian or, more accurately, quasi-Hermitian. It can be Hermitized by a similarity transformation. When the direct method, Eqs. (17) and (18), is used, the similarity transformation is determined from the metric operator $P_2(1+\omega^\dagger\omega)P_2$. The Hermitian Hamiltonian is then given by [16]

$$\overline{H}_{2\text{eff}} = [P_2(1+\omega^\dagger\omega)P_2]^{1/2} H_{2\text{eff}} [P_2(1+\omega^\dagger\omega)P_2]^{-1/2}. \tag{19}$$

When the iteration method (11) or (13) is employed, the ω operator is not determined. In previous applications [4,7,14], the Hermitization was usually done by averaging the conjugate matrix elements. However, also in this case a similarity transformation can be constructed, which Hermitizes the effective Hamiltonian. As shown in Ref. [17], if S is a matrix, which diagonalizes $H_{2\text{eff}}$, $SH_{2\text{eff}}S^{-1} = D$, then the metric operator can be expressed as $S^\dagger S$. Consequently, it follows that the Hermitized $H_{2\text{eff}}$ is obtained from

$$\overline{H}_{2\text{eff}} = [S^\dagger S]^{1/2} H_{2\text{eff}} [S^\dagger S]^{-1/2}. \tag{20}$$

Finally, the two-body effective interaction used in the shell-model calculation is determined from the two-nucleon effective Hamiltonian as $V_{2\text{eff}} = \overline{H}_{2\text{eff}} - H_{02}^{\Omega}$.

III. APPLICATION TO LIGHT NUCLEI

In this section we apply the methods for calculating the two-body effective interaction outlined in Sec. II and, with the obtained interactions, we perform no-core shell-model calculations for nuclei with $A=3$–6. We use a complete $N\hbar\Omega$ model space with, e.g., $N=8$ for the positive-parity states of ^{4}He. This means that nine major harmonic-oscillator shells may be occupied in this case. The two-nucleon model space is defined in our calculations by $N_{\max}$, e.g., for an $8\hbar\Omega$ calculation for ^{4}He $N_{\max}=8$. The restriction of the harmonic-oscillator shell occupation is given by $N_1 \leqslant N_{\max}$, $N_2 \leqslant N_{\max}$, $(N_1+N_2) \leqslant N_{\max}$. The same conditions hold for the relative $2n+l$, center-of-mass $2\mathcal{N}+\mathcal{L}$, and $2n+l+2\mathcal{N}+\mathcal{L} = N_1+N_2$ quantum numbers.

In the present calculations we use the Reid 93 nucleon-nucleon potential [18]. For ^{4}He we make a comparison with the Nijmegen II potential [18] with corrected $^1P_1$ wave [19]. We work in the isospin formalism and do not include the Coulomb interaction. The np channel interactions of Reid 93 and Nijmegen II are used.

First, let us compare the different methods for calculating the starting-energy-independent effective interaction. The KK method (11) works well for $N_{\max} \leqslant 4$. Then the convergence is achieved usually after less than 15 iterations and the model space eigenvalues differ from the full-space eigenvalues, which are of the order of 10^1–10^2 MeV, by not more than 10^{-4} MeV. Note that the reference G matrix (8b) becomes singular for $\varepsilon = E_k$. Consequently, exact eigenvalues cannot be reproduced when the reference G-matrix method is applied for calculating the G matrix. However, this singularity causes no problem when the iteration is stopped after achieving the above-mentioned precision. When the starting iteration (12) is used instead of $G(\varepsilon)$, usually a few iteration steps are saved. As to the starting energy, $\varepsilon = 0$ is a possible choice. In most calculations we used negative values for ε. For Δ a nonzero value must be chosen, and we used typically about -5 MeV. The resulting effective interaction is not dependent on these choices, and they also do not affect the number of iterations significantly. For $N_{\max} > 4$ divergence in some channels can be encountered and, moreover, the calculation becomes time consuming.

The application of the vertex-renormalization method (13) requires the G-matrix derivatives. The matrix elements of the G-matrix derivatives decrease rapidly, but, on the other hand, they are multiplied by effective-interaction matrices of increasing powers. Consequently, the overall convergence is rather slow for larger model spaces. Also the rate of convergence differs for different states. When the starting energy is chosen below the ground state energy, the fastest convergence is achieved for the lowest states, which have the largest overlap with the model space. This is the same observation as found in the model calculations [20]. The rate of convergence is very sensitive to the choice of the starting energy ε. The closer to the ground state, the faster the convergence. On the other hand, serious numerical problems occur when a higher number of iterations is required. These problems are related to the above-mentioned fact that we multiply very small numbers by very large numbers when calculating higher iterations. To achieve the same accuracy as with the previous method, often more than 30 iterations are needed, and to curb the numerical difficulties real*16 precision is neccessary. These facts make this method rather impractical. It is also difficult to apply this method for model spaces with $N_{\max} > 4$.

Let us point out that new iteration methods were suggested recently, which combine some features of both methods studied here [21]. These techniques are more involved from the computational point of view, and we did not try to use them. They may, however, remedy some of the difficulties found in our applications.

The simplest and the most straightforward way to calculate the two-body effective interaction is accomplished by solving Eq. (17) and constructing the effective Hamiltonian according to Eq. (18). The easiest way to perform the calculations is in the center-of-mass and relative-coordinate basis and afterwards to do the transformation to the two-nucleon harmonic-oscillator basis. Note that ω is diagonal in the center-of-mass quantum numbers $\mathcal{N},\mathcal{L}$ as well as in S,j,J,T. Consequently, the sum in Eq. (17) goes only over n_P,l_P for the basis states classified by $|nlSj,\mathcal{NL},JT\rangle$. An important point is the right choice of the eigenstates in the set $\mathcal{K}$. For each $S,j,\mathcal{N},\mathcal{L},J,T$ we must choose as many relative coordinate eigenstates as the allowed number of n_P,l_P combinations. These are determined from the condition $2\mathcal{N}+\mathcal{L}+2n_P+l_P\leqslant N_{\max}$. Since the harmonic-oscillator basis is infinite, we make a truncation in the Q space by keeping only the states with $n_Q\leqslant 150$. Note that $l=j\pm 1$ for the coupled channels and $l=j$ for the uncoupled channels. This method can be easily applied to calculate the effective interaction up to $N_{\max}=8$, as required in the present shell-model calculations.

To take partially into account the many-body effects neglected when using only a two-body effective interaction, we employ the recently introduced multivalued effective interaction approach [8]. In this approach different effective interactions are used for different $\hbar\Omega$ excitations. The effective interactions then carry an additional index, indicating the sum of the oscillator quanta for the spectators, $N_{\rm sps}$, defined by

$$N_{\rm sps}=N_{\rm sum}-N_\alpha=N'_{\rm sum}-N_\gamma, \tag{21}$$

where $N_{\rm sum}$ and $N'_{\rm sum}$ are the total oscillator quanta in the initial and final many-body states, respectively, and N_α and N_γ are the total oscillator quanta in the initial and final two-nucleon states $|\alpha\rangle$ and $|\gamma\rangle$, respectively. Different sets of the effective interaction are determined for different model spaces characterized by $N_{\rm sps}$ and defined by the projection operators

$$Q_2(N_{\rm sps})=\begin{cases}0 & \text{if } N_1+N_2\leqslant N_{\max}-N_{\rm sps},\\ 1 & \text{otherwise,}\end{cases} \tag{22a}$$

$$P_2(N_{\rm sps})=1-Q_2(N_{\rm sps}). \tag{22b}$$

This multivalued effective interaction approach is superior to the traditional single-valued effective interaction, as confirmed also in a model calculation [9].

The shell-model diagonalization is performed by using the many-fermion-dynamics shell-model code [22]. We present the results for $A=3$–6 nuclei in Tables I–V. It has been observed earlier [7] and it is apparent in the present calculations as well that, when the effective interaction is derived using the Lee-Suzuki method, the interaction becomes too strong and leads to overbinding of nuclei. The problem is not in the calculational method but rather in the fact that the original two-nucleon Hamiltonian (5) is flawed if $P_2\neq 1$. The difficulty is that while the relative-coordinate harmonic-oscillator auxiliary potential is exactly canceled in Eq. (2), it is not fully canceled when the effective interaction is derived from the two-nucleon Hamiltonian (5). This can be seen, for example, when the nucleon-nucleon interaction is switched off. Then from Eq. (5) we obtain an effective interaction derived from the relative-coordinate harmonic-oscillator potential, which will be different from the model-space part of the harmonic-oscillator potential, appearing in Eq. (4). Clearly, the Q_2-space part of the relative-coordinate harmonic-oscillator potential is responsible for this effect. In order to reduce this spurious effect of the auxiliary potential on the effective interaction, we introduce an *ad hoc* modification of the relative-coordinate two-nucleon Q-space part of the auxiliary potential as follows:

$$\begin{aligned}H^{\Omega}_{\rm 2rel}=&\frac{\vec{q}^2}{2\mu}+P_2\frac{A-2}{2A}\mu\Omega^2\vec{r}^2P_2+P_2k_Q\frac{A-2}{2A}\mu\Omega^2\vec{r}^2Q_2\\&+Q_2k_Q\frac{A-2}{2A}\mu\Omega^2\vec{r}^2P_2+Q_2k_Q\frac{A-2}{2A}\mu\Omega^2\vec{r}^2Q_2\\&+(1-k_Q)\frac{1}{2}\hbar\Omega\sqrt{\frac{A-2}{A}}(N_{\max}+2)Q_2+V(\vec{r}).\end{aligned} \tag{23}$$

Here we have introduced a constant $k_Q\leqslant 1$; for $k_Q=1$, we get the original Hamiltonian appearing in Eq. (6). Moreover, for $A=2$ the harmonic-oscillator dependence vanishes and for $P\rightarrow 1$ the relative-coordinate part of the Hamiltonian (6) is recovered. In Eq. (23) the Q-space harmonic-oscillator potential is made more shallow and is shifted. The shift is such that the P-space and the Q-space potentials are equal for $\vec{r}^2=\frac{1}{2}(\langle\vec{r}^2\rangle_{N_{\max}}+\langle\vec{r}^2\rangle_{N_{\max}+1})$, with this mean value determined for the eigenstates of the relative-coordinate harmonic-oscillator Hamiltonian appearing in Eq. (6). In this modified Hamiltonian (23), a quasiparticle scattered into the Q space ''feels'' a weaker auxiliary potential. Note that an alternative method by Krenciglowa *et al.* [28] for deriving the G matrix, as opposed to that we employ here [10], uses plane-wave-type intermediate Q-space states, that is, no auxiliary potential at all. For a recent review of this approach, see Ref. [29]. Our present modification, in fact, brings those two methods closer together. We solve the Schrödinger equation with the Hamiltonian (23) by diagonalization in a harmonic-oscillator basis characterized by $b=\sqrt{\hbar/\mu\Omega}$ with the radial quantum number $n=0,\ldots,150$. The error caused by this truncation of the harmonic-oscillator basis can be estimated for $k_Q=1$, when the system can be solved as a differential equation. We found that the low-lying eigenvalues obtained in the two calculations do not differ by more than 10^{-3} MeV and in most cases by much less. The lowest eigenvalues are typically of the order of 10^1 MeV. The diagonalization cannot be used for hard-core nucleon-nucleon potentials, but for the soft-core Reid 93 and Nijmegen II potentials the interaction matrix elements can be evaluated straightforwardly. Note that the Hamiltonian (23) depends on $N_{\max}$ and the projection operators. When the multivalued ef-

TABLE I. Experimental and calculated binding energy in MeV, point proton radius in fm, and magnetic moment in μ_N, for ^{3}H. The ground state has $J^\pi = \frac{1}{2}^+$. The $8\hbar\Omega$ calculation results are presented. Different k_Q choices correspond to different two-nucleon Hamiltonians, from which the multivalued effective interaction is calculated, as explained in the text. The Reid 93 nucleon-nucleon potential is used, and the harmonic-oscillator parameter is taken to be $\hbar\Omega = 19.2$ MeV. The exact, calculated binding energy for this potential is 7.63 MeV. The free nucleon g factors were used. The experimental values are taken from Ref. [23].

^{3}H	$k_Q=1$	$k_Q=0.6$	Expt.
E_B	8.739	7.674	8.482
$\sqrt{\langle r_p^2\rangle}$	1.540	1.600	1.41–1.62
μ	2.638	2.634	2.979

fective interaction is calculated, solutions are found only for projectors and $N_{\max}$ corresponding to $N_{\rm sps}=0$. The value $N_{\max}=8$ is used in most calculations. Using these solutions, all required sets of effective interactions are constructed.

The question arises if the modification we introduced in Eq. (23) may not cause center-of-mass spurious contamination of the physical states. We note that the modification is done only in the Q-space part of the auxiliary potential and, most importantly, with regard to the two-nucleon relative coordinate. In conjuction with this, our choice of the two-nucleon model space as well as the complete $N\hbar\Omega$ model space for the many-nucleon states prevents the center-of-mass contamination of physical states. We have tested numerically for possible spurious center-of-mass contaminations by varying the parameter β, introduced in Eq. (4), in calculations for several systems and found that the physical states remain unchanged for different choices of β, including $\beta=0$, even if $k_Q\neq 1$.

We note that the free (or bare) values of the nucleon charges are used for calculating mean values of different operators.

In Table I we present results of the $8\hbar\Omega$ calculation for ^{3}H with $\hbar\Omega=19.2$ MeV as suggested by the formula [30] (in units of MeV)

$$\hbar\Omega = 45A^{-1/3} - 25A^{-2/3}. \tag{24}$$

We observe that the calculation, using the effective interaction derived from the Hamiltonian (5) or, equivalently, $k_Q=1$ in Eq. (23), overbinds the system in comparison with both the experimental value (8.482 MeV) and the exact result for the Reid 93 calculation (7.63 MeV) [31]. Our aim should be to reproduce the result of the exact calculation. To achieve that we varied the parameter k_Q in Eq. (23). The value $k_Q=0.6$ gives reasonable agreement. We keep this value for all other calculations, so that a meaningful comparison of binding energies can be obtained.

In Table II the calculated results for ^{4}He are presented, where we have used $8\hbar\Omega$ for the positive-parity states and $7\hbar\Omega$ for the negative-parity states. The value $\hbar\Omega=18.4$ MeV, obtained from Eq. (24) is employed. The results for calculations with $k_Q=1$ and $k_Q=0.6$, using the Reid 93 potential, are shown, as well as calculations with $k_Q=0.6$, using the Nijmegen II potential. We observe that both potentials give almost identical results. The effective interaction derived using the unmodified relative-coordinate two-body Hamiltonian overbinds the system. On the other hand, the calculation with the modified Hamiltonian gives very reasonable agreement with the experimental results. Unlike the experimental spectrum we still get the $2\hbar\Omega\ 0^+$ state above the $1\hbar\Omega\ 0^-$; however, the discrepancy is reduced considerably in comparison with previous calculations [6] and most of the

TABLE II. Experimental and calculated binding energy, point proton radius in fm and excitation energies $E_x(J^\pi,T)$ for ^{4}He. All energies are in MeV. The $8\hbar\Omega$ ($\pi=+$) and $7\hbar\Omega$ ($\pi=-$) calculation results are presented. Different k_Q choices correspond to different two-nucleon Hamiltonians, from which the multivalued effective interaction was calculated, as explained in the text. Both the Reid 93 and Nijmegen II nucleon-nucleon potentials are used for comparison purposes. The harmonic-oscillator parameter is taken to be $\hbar\Omega=18.4$ MeV. The experimental values are taken from Refs. [24,25].

^{4}He	Reid 93 $k_Q=1$	Reid 93 $k_Q=0.6$	Nijmegen II $k_Q=0.6$	Expt.
E_B	31.115	27.408	27.499	28.296
$\sqrt{\langle r_p^2\rangle}$	1.378	1.434	1.432	1.46
$E_x(0_1^+,0)$	0	0	0	0
$E_x(0_2^+,0)$	24.009	21.619	21.724	20.21
$E_x(0_1^-,0)$	23.506	21.290	21.402	21.01
$E_x(2_1^-,0)$	25.118	22.852	22.948	21.84
$E_x(2_1^-,1)$	26.544	24.056	24.125	23.33
$E_x(1_1^-,1)$	26.874	24.263	24.325	23.64
$E_x(1_1^-,0)$	27.763	25.113	25.205	24.25
$E_x(0_1^-,1)$	27.940	25.247	25.325	25.28
$E_x(1_2^-,1)$	28.154	25.419	25.487	25.95

TABLE III. Experimental and calculated binding energy, point proton radius in fm, magnetic moment in μ_N, quadrupole moment in e fm^2, and excitation energies $E_x(J^\pi,T)$ for ^{5}He. All energies are in MeV. The $7\hbar\Omega$ ($\pi=+$) and $6\hbar\Omega$ ($\pi=-$) calculation results are presented. Different k_Q choices correspond to different two-nucleon Hamiltonians, from which the multivalued effective interaction was calculated, as explained in the text. The Reid 93 nucleon-nucleon potential is used, and the harmonic-oscillator parameter is taken to be $\hbar\Omega=17.8$ MeV. The calculated $\frac{3}{2}^+_2$ state is associated with the experimental $\frac{3}{2}^+$ state as it is dominated by the $(0s)^3(0p)^2$ configuration. See also Figs. 1 and 2. The experimental values are taken from Ref. [26].

^{5}He	$k_Q=1$	$k_Q=0.6$	Expt.
E_B	30.454	26.105	27.402
$\sqrt{\langle r_p^2\rangle}$	1.531	1.597	NA[a]
μ	-1.845	-1.844	NA
Q	-0.437	-0.489	NA
$E_x(\frac{3}{2}^-_1,\frac{1}{2})$	0	0	0
$E_x(\frac{1}{2}^-_1,\frac{1}{2})$	2.537	2.026	4 ± 1
$E_x(\frac{1}{2}^+_1,\frac{1}{2})$	4.062	3.113	NA
$E_x(\frac{3}{2}^+_1,\frac{1}{2})$	9.503	8.099	NA
$E_x(\frac{5}{2}^+_1,\frac{1}{2})$	9.520	8.172	NA
$E_x(\frac{3}{2}^-_2,\frac{1}{2})$	11.200	10.413	NA
$E_x(\frac{1}{2}^-_2,\frac{1}{2})$	15.049	14.025	NA
$E_x(\frac{1}{2}^+_2,\frac{1}{2})$	20.931	18.652	NA
$E_x(\frac{3}{2}^+_2,\frac{1}{2})$	21.378	19.454	16.75

[a]Not available.

states compare better with the experiment data than in the recent calculation with a multivalued effective interaction [8].

The calculation for ^{5}He was performed for several values of $\hbar\Omega$ and different model spaces in order to study the dependence of different states on these quantities. In Table III we show the $7\hbar\Omega$ ($\pi=+$) and $6\hbar\Omega$ ($\pi=-$) results, respectively, using $\hbar\Omega=17.8$ MeV obtained from Eq. (24). The controversy regarding the shell-model calculations for this nucleus has to do with the nature of the excited states [32]. In the standard shell-model formulation, also employed here, the center of mass of the nucleus is bound in a harmonic-oscillator potential, and so all states are bound. However, they do not necessarily belong to the internal excitations of the studied nucleus. They may as well correspond to, e.g., a two-cluster configuration. One would expect that such states are more sensitive to the variation of the model space size and the harmonic-oscillator binding potential [33]. In Fig. 1 we present the $\hbar\Omega$ dependence of the ^{5}He states calculated in the $7\hbar\Omega$ ($\pi=+$) and $6\hbar\Omega$ ($\pi=-$) model spaces, respectively, by using the effective interaction obtained for $k_Q=0.6$ and $N_{\max}=8$ in Eq. (23). Note that only three experimental states are known in this nucleus. Also the excitation energy of the $\frac{1}{2}^-$ state is determined with a large error. For comparison, in Fig. 2 results for the $5\hbar\Omega$ ($\pi=+$) and $4\hbar\Omega$ ($\pi=-$) model spaces, respectively, are presented. The effective interaction for this calculation has been derived from Eq. (23) with the same $k_Q=0.6$ but different $N_{\max}=6$. We observe a large sensitivity for the higher excited states on changes in $\hbar\Omega$ with the exception of $\frac{3}{2}^+_2$. This state, dominated by the $(0s)^3(0p)^2$ configuration, is a good candidate for the experimental $\frac{3}{2}^+$ state. Note also the significant shifts of the excited states, again with the exception of $\frac{3}{2}^+_2$ and $\frac{1}{2}^-_1$, downwards in energy, when the model space is enlarged. Even if we cannot draw a definitive conclusion, these facts indicate that excited states obtained in the calculation, but unobserved, may be states, which do not correspond to ^{5}He internal excitations.

The calculated results for ^{6}Li are presented in Table IV. A $6\hbar\Omega$ calculation was performed for the positive-parity states using $\hbar\Omega=17.2$ MeV obtained from Eq. (24). Again the effective interaction, derived from the Hamiltonian (5), is too strong and overbinds the system. The calculation with the modified Hamiltonian (23) gives very reasonable agreement with experiment for all properties shown. In addition to

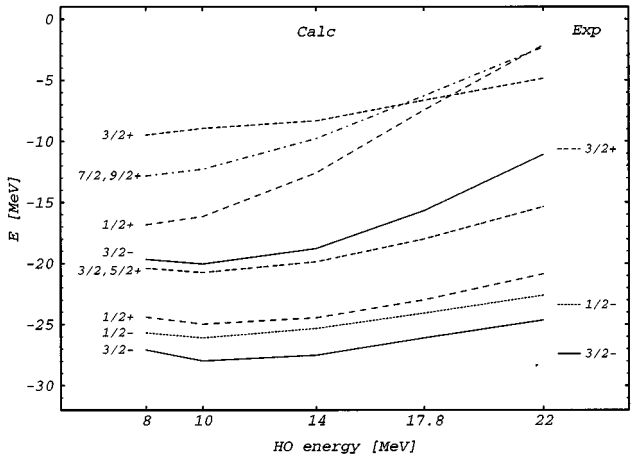

FIG. 1. Energy dependence for the ^{5}He states on the harmonic-oscillator energy $\hbar\Omega$ in a full $6\hbar\Omega$ and $7\hbar\Omega$ calculation. Only the three lowest negative-parity states are shown. The positive-parity states $\frac{3}{2}^+,\frac{5}{2}^+$ and $\frac{7}{2}^+,\frac{9}{2}^+$ have very close energies. Therefore, only single lines for these pairs of states are presented. The second $\frac{3}{2}^+$ state is dominated by the s^3p^2 configuration and should correspond to the experimental $\frac{3}{2}^+$ state. For further description of the calculation, see the text.

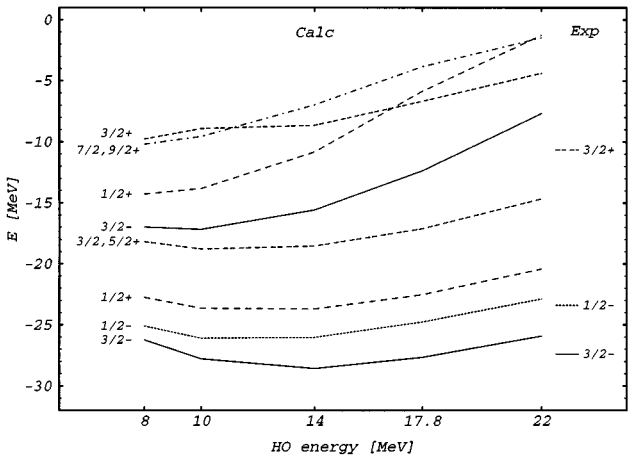

FIG. 2. Energy dependence for the ^{5}He states on the harmonic-oscillator energy $\hbar\Omega$ in a full $4\hbar\Omega$ and $5\hbar\Omega$ calculation. See Fig. 1 for the details.

the experimental states presented in the Table IV, another $J^\pi=3^+,T=0$ state with the excitation energy 15.8 MeV is known. The lowest $J^\pi=3^+,T=0$ $2\hbar\Omega$ state obtained in our $k_Q=0.6$ calculation has an energy of 13.840 MeV, with a main configuration of $(0s)^4(0p)^1(1p0f)^1$. Another candidate for this experimental state may be the calculated state with an excitation energy of 18.378 MeV, dominated by the configurations $(0s)^4(1s0d)^2$ and $(0s)^3(0p)^2(1s0d)^1$. Likely, the latter state may be more stable against model space and $\hbar\Omega$ variations. We also performed a $5\hbar\Omega$ calculation for the negative-parity states of ^{6}Li. The lowest calculated state is $J^\pi=2^-,T=0$ with an excitation energy 9.135 MeV, followed by $J^\pi=1^-,T=0$ (E_x=9.335 MeV) and $J^\pi=0^-,T=0$ (E_x=11.372 MeV). Such states have not been observed experimentaly.

In Table V we present the ^{6}He characteristics. As isospin symmetry is not broken in the present calculations, the energies are the same as those for ^{6}Li with $T=1$. In addition, the proton and neutron radii are evaluated. Reasonable agreement with the experimantal values is found.

Contrary to the previous no-core shell-model calculations [6,8], the effective interaction used in the present calculations does not contain a parameter Δ adjusted for each nucleus in order to get a reasonable binding energy. Besides the model-space size, the present calculations depend only on the harmonic-oscillator frequency $\hbar\Omega$ and on the parameter k_Q, appearing in the relative-coordinate two-nucleon Hamiltonian (23), which distinguishes the structure of the P space from that of the Q space. For the results presented in Tables I–V, we chose $\hbar\Omega$ according to formula (24) and k_Q was fixed to reproduce the result of the exact ^{3}H calculation. Consequently, our calculations contain no variable parameters and meaningful comparisons can be made between our calculated binding energies and the quantities derived from them and the experimental values as well as the results of other calculations.

In this regard, we note the recent calculation of valence energies of ^{6}He and ^{6}Li and the neutron separation energy of ^{5}He, using the two-frequency shell-model approach [34]. For example, our calculation with $k_Q=0.6$ and the Reid 93 potential gives for the neutron separation energy of ^{5}He, $E_{\rm sp}=E_B(^5{\rm He})-E_B(^4{\rm He})=-1.303$ MeV to be compared with the experimental value of -0.894 MeV. Similarly, the valence energy of ^{6}He is found to be $E_{\rm val}(^6{\rm He})=-[E_B(^6{\rm He})+E_B(^4{\rm He})-2E_B(^5{\rm He})]=-3.151$ MeV, compared with the experimental -2.761 MeV. Furthermore, $E_{\rm val}(^6{\rm Li})=-[E_B(^6{\rm Li})+E_B(^4{\rm He})-E_B(^5{\rm He})-E_B(^5{\rm Li})]=-6.845$ MeV, where we used $E_B(^5{\rm Li})=E_B(^5{\rm He})=26.105$ MeV from Table III, as the Coulomb contributions, not taken into account in the calculations, more or less can-

TABLE IV. Experimental and calculated binding energy, point proton radius in fm, magnetic moment in μ_N, quadrupole moment in e fm^2, and excitation energies $E_x(J^\pi,T)$ for ^{6}Li. All energies are in MeV. The $6\hbar\Omega$ calculation results are presented. Different k_Q choices correspond to different two-nucleon Hamiltonians, from which the multivalued effective interaction was calculated, as explained in the text. The Reid 93 nucleon-nucleon potential is used, and the harmonic-oscillator parameter is chosen to be $\hbar\Omega=17.2$ MeV. Only the states dominated by the $0\hbar\Omega$ configuration are presented. See the text for the discussion of other states. The experimental values are taken from Refs. [25,26].

^{6}Li	$k_Q=1$	$k_Q=0.6$	Expt.
E_B	37.532	31.647	31.995
$\sqrt{\langle r_p^2\rangle}$	1.995	2.097	2.42
μ	0.839	0.839	0.822
Q	0.027	-0.052	-0.082
$E_x(1_1^+,0)$	0	0	0
$E_x(3_1^+,0)$	2.368	2.398	2.19
$E_x(0_1^+,1)$	4.301	3.695	3.56
$E_x(2_1^+,0)$	4.966	4.438	4.31
$E_x(2_1^+,1)$	6.878	6.144	5.37
$E_x(1_2^+,0)$	7.232	6.277	5.65
$E_x(2_2^+,1)$	10.641	9.333	NA
$E_x(1_1^+,1)$	11.442	10.019	NA
$E_x(1_3^+,0)$	11.847	10.467	NA
$E_x(0_2^+,1)$	13.866	12.050	NA

TABLE V. Experimental and calculated binding energy, point proton and neutron radius in fm, and excitation energies $E_x(J^\pi,T)$ for ^{6}He. All energies are in MeV. The presented results are for $6\hbar\Omega$ and are performed as described in Table IV. The experimental values are taken from Refs. [26,27].

^{6}He	$k_Q=1$	$k_Q=0.6$	Expt.
E_B	33.230	27.953	29.269
$\sqrt{\langle r_p^2\rangle}$	1.629	1.707	1.72
$\sqrt{\langle r_n^2\rangle}$	2.196	2.317	2.59
$E_x(0_1^+,1)$	0	0	0
$E_x(2_1^+,1)$	2.577	2.449	1.80
$E_x(2_2^+,1)$	6.339	5.638	NA
$E_x(1_1^+,1)$	7.140	6.324	NA
$E_x(0_2^+,1)$	9.565	8.355	NA

cel. Here the experimental value is -6.559 MeV. We observe good agreement of these quantities with the experimental values, in fact, better than that obtained in Ref. [34]. Apparently, the reason for these improved results is the size of the model space, which is much larger in our calculations.

In Ref. [32] concerns were raised about the stability of ^{6}Li to the $\alpha+d$ threshold in previous no-core calculations [6]. From the present results we deduce that ^{6}Li is bound against this threshold by 1.314 MeV, compared with the experimental value of 1.474 MeV. Note that the deuteron is treated exactly in our formalism, $E_B(d)=2.2246$ MeV. To arrive at the present number, we used the Coulomb energy contributions to binding energy $E_C(Z\equiv 2)=-0.76$ MeV and $E_C(Z\equiv 3)=-1.46$ MeV. Another issue raised in Ref. [32] was the sign of the quadrupole moment of ^{6}Li. As in the previous no-core calculations [6,8], we also get the sign correctly in our $k_Q=0.6$ calculation. Clearly, this is a consequence of a reasonable effective interaction and a large enough model space.

IV. CONCLUSIONS

In the present paper we have presented different ways of constructing a starting-energy-independent two-body effective interaction. In particular, we studied the Lee-Suzuki similarity transformation method and compared two different iteration schemes for obtaining a solution, the vertex renormalization method and the Krenciglowa-Kuo method. When applying the vertex renormalization method, we obtained the derivatives of the G matrix exactly by using the derivatives of the reference G matrix. A third approach involved a direct calculation of the transformation operator ω. When the convergence conditions of the iteration methods are satisfied, all three approaches lead to the same two-body effective interaction. Our conclusion is that, for the large model spaces that we employ, the only viable option is the direct calculation method. For large model spaces ($N_{\max}>4$), the iteration methods either fail to converge or the calculations are time consuming or both.

Unlike in most previous applications, where the non-Hermitian effective interaction was Hermitized by averaging the conjugate matrix elements, we Hermitize the effective interaction exactly using a similarity transformation. It was demonstrated in Ref. [35] that the averaging is a good approximation for the Hermitian sd and pf effective interactions. We observe here, however, that for large model spaces, like those we employ, the non-Hermiticity could be significant. It is certainly preferable to work with the exactly Hermitized interaction.

Employing the derived effective interaction, we have performed shell-model calculations, in which up to nine major harmonic-oscillator shells may be occupied. In order to take into account part of the many-body effects, we utilized the new multivalued effective interaction approach [8]. The results for no-core, full $N\hbar\Omega$ calculations are given for nuclei with $A=3$–6. The effective interaction was derived from the Reid 93 nucleon-nucleon potential, but calculations were also made with Nijmegen II potential for comparison. As observed earlier [7], when the Lee-Suzuki method is applied for a two-nucleon system with a harmonic-oscillator auxiliary potential, the resulting effective interaction is too strong and leads to overbinding of the many-body system. This problem is caused by incomplete cancellation of the relative coordinate part of the auxiliary potential. To mend this flaw, we introduced a modification of the Q-space part of the relative-coordinate two-nucleon Hamiltonian, from which the effective interaction is calculated. In effect this weakens the auxiliary potential in the Q space.

In the present calculations, besides the model-space size, the only free parameters are the harmonic-oscillator frequency $\hbar\Omega$ and the parameter modifing the two-nucleon Hamiltonian, as discussed above. The latter parameter was fixed from the ^{3}H binding energy calculation (fitted to the result of an exact ^{3}H calculation) and $\hbar\Omega$ was taken from the phenomenological formula (24). Hence, unlike previous no-core calculations, we are able to compare, for nuclei other than ^{3}H, quantities derived from binding energies, such as valence energies, with experiment.

For most calculated characteristics we found good agreement with the experimental values. In agreement with the previous observation [5], we found that the Reid 93 and Nijmegen II potentials give very similar results. The question of low-lying positive-parity states in ^{5}He was also investigated. We observed that the calculated low-lying positive-parity states have not converged, regarding changes in the model-space size and variations in $\hbar\Omega$. This may indicate that they do not correspond to internal excitations of ^{5}He. However, we are not in a position to make a conclusive statement concerning this issue.

Because we derive the transformation operator ω explic-

itly in our calculations, we are able to use it for calculating any effective operator, employing the approaches discussed in Refs. [36,37], in a similar way as in our model calculations [9]. Besides calculating other effective operators, we also intend to extend the calculations to larger A.

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