Microscopic origins of effective charges in the shell model

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We use a large-scale $6\hbar\Omega$ calculation for ^{6}Li with microscopically derived two-body interaction to construct the $0\hbar\Omega$ $0p$ shell effective Hamiltonian, electric quadrupole, and magnetic dipole operators. While the $E2$ and $M1$ $6\hbar\Omega$ operators are one-body operators with free nucleon charges, the effective operators are two-body operators with substantially different renormalization for the isoscalar and isovector matrix elements, especially for the $E2$ operator. We show that these operators can be very well approximated by one-body operators provided that effective proton *and* neutron charges are used. The obtained effective charges are compatible with those used in phenomenological shell-model studies. The two-body part of the effective operators is estimated. [S0556-2813(97)50202-0]

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Considerable effort has been devoted to derive the effective interaction used in the shell-model calculations from the nucleon-nucleon interaction [1–3]. On the other hand, much less work has been done to understand the effective operators employed in calculating different nuclear, usually electromagnetic, properties. In particular, a microscopic derivation of effective operators has been only partially successful. It is well known that effective proton and neutron charges must be employed to describe the $E2$ transitions and moments. These charges are quite different from the free nucleon charges, typically the values of $e_{\text{eff}}^{\text{p}}\approx 1.5e$ and $e_{\text{eff}}^{\text{n}}\approx 0.5e$ are obtained for both light and heavy nuclei. Attempts to derive these charges microscopically, usually by perturbation [3], or by an ''expanded shell-model'' approach [4], yielded much smaller values. It should be noted that these effective charges correspond to a severely truncated single-major-shell, or $0\hbar\Omega$, space. The question arises as to what causes the nucleon properties to change so significantly, is it mostly the result of the space truncation or the fact that nucleons are bound? Also the non-nucleonic degrees of freedom may play an important role. Other interesting questions are: how important are the higher than one-body parts of the effective operators and what is the j dependence of effective charges?

In this contribution we investigate how severe space truncation affects the electromagnetic operators. We use a large-space $6\hbar\Omega$ shell-model calculation for ^{6}Li, with a microscopically derived two-body interaction, to construct an effective Hamiltonian and effective electromagnetic operators, which will exactly reproduce the $6\hbar\Omega$ results in the $0p$ shell for the $(0s)^4(0p)^2$ dominated states. This enables us to compare the resulting effective operators with the bare one-body $0p$-shell operators and to extract the relevant effective charges, which allow us to determine the amount of renormalization, to study their j dependence, and, eventually, to quantify the two-body content of the effective operators. Also we perform the same derivation from the corresponding $4\hbar\Omega$ calculation to study the dependence on the space size and compare the rate of convergence for the effective Hamiltonian and the effective operators.

Recently, large-basis no-core shell-model calculations have been performed [5,6]. 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 microscopically from the nucleon-nucleon interaction for a system of two nucleons and subsequently used in the many-particle calculations. To take into account a part of the many-body effects, a multivalued effective interaction approach was introduced [6], which uses different sets of the effective interaction for different $\hbar\Omega$ excitations. In the latest application of the no-core approach, we derived starting-energy-independent Hermitian two-body effective interactions from the Reid 93 nucleon-nucleon potential [7] and applied them in the multivalued approach to $A=3-6$ nuclei [8]. In this study we use the results of this calculation for ^{6}Li presented in the third column of Table IV of Ref. [8]. The many-particle calculation was done using the many-fermion-dynamics shell-model code [9] in the m scheme with dimensions approaching 2×10^5. As in the previous large-scale no-core shell-model calculations [5,6], a reasonable description of the electromagnetic properties has been achieved using free nucleon charges. Our aim here is to study the renormalization of these operators, when the model space is severely truncated.

For the $0\hbar\Omega$ dominated states of ^{6}Li shown in Table IV of Ref. [8], it is possible to formulate an equivalent description purely in the $0p$ shell. We may divide the basis states of the $6\hbar\Omega$ calculation into two subspaces, using the projectors P and Q, $P+Q=1$. Here the P space is spanned by the states $|(0s)^4(0p)^2\rangle$. There are 10 such states in the $M_J=0$ m scheme calculation and 8 in the $M_J=1$ calculation, respectively. The Q space is then formed by the rest of the almost 200 000 states. The effective P-space Hamiltonian may be constructed by employing the Lee-Suzuki starting-energy independent similarity transformation method [10], which gives the effective Hamiltonian $PH_{\text{eff}}P=PHP+PHQ\omega P$, with the transformation operator ω satisfying $\omega=Q\omega P$. In the case when the full space eigenvectors are known, like in our situation, this operator may be obtained directly. Let us denote the P space states as $|\alpha_P\rangle$,

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and those which belong to the Q space, as $|\alpha_Q\rangle$. Then the Q space components of the eigenvector $|k\rangle$ of the full-space Hamiltonian can be expressed as a combination of the P-space components with the help of the operator ω

$$\langle\alpha_Q|k\rangle=\sum_{\alpha_P}\langle\alpha_Q|\omega|\alpha_P\rangle\langle\alpha_P|k\rangle. \tag{1}$$

If the dimension of the model space is d_P, we may choose a set $\mathcal{K}$ of d_P eigenevectors $|k\rangle$, for which the relation (1) will be satisfied. In our case we choose those states, which have the dominant $0\hbar\Omega$ component. Under the condition that the $d_P\times d_P$ matrix $\langle\alpha_P|k\rangle$ for $|k\rangle\in\mathcal{K}$ is invertible, which is satisfied in the present application, the operator ω can be determined from Eq. (1). Consequently, the effective Hamiltonian can be constructed as follows

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

It should be noted that $P|k\rangle=\Sigma_{\alpha_P}|\alpha_P\rangle\langle\alpha_P|k\rangle$ for $|k\rangle\in\mathcal{K}$ is a right eigenvector of Eq. (2) with the eigenvalue E_k. The Hamiltonian (2) is, in general, non-Hermitian, or more accurately quasi-Hermitian. It can be Hermitized by a similarity transformation, which is determined from the metric operator $P(1+\omega^\dagger\omega)P$. The Hermitian Hamiltonian is then given by [11]

$$\overline{H}_{\rm eff}=[P(1+\omega^\dagger\omega)P]^{1/2}H_{\rm eff}[P(1+\omega^\dagger\omega)P]^{-1/2}. \tag{3}$$

Similarly, a corresponding effective operator $\hat{O}_{\rm eff}$ can be constructed for any full space, e.g., electromagnetic, operator $\hat{O}$ so that it exactly reproduces the full space results for the P-space eigenstates. A double-similarity transformation [12] leads to the P-space operator associated with the Hamiltonian (2) in the form $\hat{O}_{\rm eff}=[P(1+\omega^\dagger\omega)P]^{-1}(P+P\omega^\dagger Q)\hat{O}(P+Q\omega P)$. The operator associated with the Hermitian P-space Hamiltonian (3) is then obtained as [12,13]

$$\overline{O}_{\rm eff}=[P(1+\omega^\dagger\omega)P]^{-1/2}(P+P\omega^\dagger Q)\hat{O}(P+Q\omega P)\times[P(1+\omega^\dagger\omega)P]^{-1/2}. \tag{4}$$

Using the Eqs. (1)–(3), we constructed the effective Hamiltonian, whose matrix elements, after performing the transformation from m scheme to JT basis, are presented in Table I. In the same table the well-known Cohen-Kurath matrix elements [14] are shown. These were obtained by a least-square fit to experimental binding energies, relative to ^{4}He, and excitation energies of $A=6-16$ nuclei. To make a meaningful comparison, the calculated binding energy of ^{4}He, 27.408 MeV, obtained by using the same no-core approach in the $8\hbar\Omega$ space [8], was added to the diagonal matrix elements of our Hamiltonian. Note that by diagonalizing the Hamiltonian in Table I, we get the same excitation energies as those from the $6\hbar\Omega$ calculation given in the third column of Table IV of Ref. [8]. We also present the effective Hamiltonian obtained in the same way from a $4\hbar\Omega$ calculation. Note that the dimension of the $4\hbar\Omega$ calculation is more than an order of magnitude smaller than that of the $6\hbar\Omega$ calculation. The effective interaction used in this calculation was obtained from the $6\hbar\Omega$ multivalued interaction by leaving out the set corresponding to the $6\hbar\Omega$ space. Let us mention that the change in the low-lying eigenenergies in the two calculations is not substantial and the ordering of levels is identical. We observe that our calculated matrix elements differ in some cases from the phenomenological ones. Let us point out, however, that our matrix elements provide a better description of ^{6}Li states than those of Cohen-Kurath. This can be understood as the latter matrix elements were fitted to a large number of nuclei across the entire $0p$ shell.

TABLE I. The $0p$-shell effective Hamiltonian matrix elements, in MeV, obtained from $6\hbar\Omega$, second column, and from $4\hbar\Omega$, third column, calculation for ^{6}Li. The calculated binding energy of ^{4}He, 27.408 MeV, obtained by using the same method in the $8\hbar\Omega$ space [8], was added to the diagonal matrix elements in order to make a meaningful comparison with the Cohen-Kurath phenomenological matrix elements [14], presented in the fourth column.

$\langle 2j_12j_2,JT\|H\|2j_32j_4,JT\rangle$	Eff	Eff-4	CK 6-16
$\langle 11,01\|H\|11,01\rangle$	6.772	7.165	4.88
$\langle 11,01\|H\|33,01\rangle$	−2.756	−3.201	−5.32
$\langle 33,01\|H\|33,01\rangle$	0.493	−0.970	0.52
$\langle 11,10\|H\|11,10\rangle$	3.999	4.202	0.28
$\langle 11,10\|H\|13,10\rangle$	−0.776	−0.988	−1.39
$\langle 13,10\|H\|13,10\rangle$	−0.788	−1.333	−2.64
$\langle 11,10\|H\|33,10\rangle$	2.086	2.464	1.09
$\langle 13,10\|H\|33,10\rangle$	−4.107	−4.708	−4.02
$\langle 33,10\|H\|33,10\rangle$	0.815	−0.707	0.12
$\langle 13,11\|H\|13,11\rangle$	5.780	5.308	4.76
$\langle 13,20\|H\|13,20\rangle$	0.199	−1.366	−0.32
$\langle 13,21\|H\|13,21\rangle$	4.303	3.514	2.76
$\langle 13,21\|H\|33,21\rangle$	1.377	1.613	2.21
$\langle 33,21\|H\|33,21\rangle$	2.694	1.162	2.61
$\langle 33,30\|H\|33,30\rangle$	−1.842	−3.771	−3.42

Our primary aim is to derive $0p$-shell effective electromagnetic operators. In the full-space calculation, we employed the one-body $E2$ and $M1$ operators

$$T^{(E2)}=e^{\rm p}\sum_{i=1}^{A}\left(\tfrac{1}{2}+t_{zi}\right)r_i^2Y^{(2)}(\Theta_i)+e^{\rm n}\sum_{i=1}^{A}\left(\tfrac{1}{2}-t_{zi}\right)r_i^2Y^{(2)}(\Theta_i), \tag{5a}$$

$$T^{(M1)}=\sqrt{3/4\pi}\,\mu_N\sum_{i=1}^{A}\left[\left(\tfrac{1}{2}+t_{zi}\right)(g_l^{\rm p}\mathbf{l}_i+g_s^{\rm p}\mathbf{s}_i)+\left(\tfrac{1}{2}-t_{zi}\right)(g_l^{\rm n}\mathbf{l}_i+g_s^{\rm n}\mathbf{s}_i)\right], \tag{5b}$$

with the free nucleon charges $e^{\rm p}=e$, $e^{\rm n}=0$ and free nucleon g factors $g_l^{\rm p}=1$, $g_l^{\rm n}=0$, $g_s^{\rm p}=5.586$, and $g_s^{\rm n}=-3.826$. The P-space operators are constructed by the application of Eq. (4). We calculate the P-space $T^{(E2)}$ operator and separately

TABLE II. Selected reduced matrix elements of the proton $E2$, in $\hbar/m\Omega$, and $M1$, in μ_N, operators. Here, $\langle\hat{O}\rangle\equiv\langle 2j_1 2j_2, J_1T_1|\hat{O}|2j_3 2j_4, J_3T_3\rangle$. In the second column the $0p$-shell effective operator matrix elements, obtained from the $6\hbar\Omega$ calculation for ^{6}Li, are presented. The third column shows the corresponding proton one-body (ob) operator matrix elements. The fourth and fifth columns display the matrix elements of the one-body operators with j-dependent and j-independent effective charges, respectively. These operators are combinations of one-body proton *and* neutron operators.

$\langle\hat{O}\rangle$	Eff	ob	ob eff-j	ob eff
$\langle 11,10|E2|13,20\rangle$	5.916	2.739	5.539	5.179
$\langle 11,10|E2|13,21\rangle$	−3.101	−2.739	−3.256	−3.184
$\langle 13,20|E2|13,21\rangle$	2.137	2.092	2.321	2.432
$\langle 13,21|E2|13,21\rangle$	−3.612	−2.092	−3.605	−3.956
$\langle 13,10|E2|33,21\rangle$	−2.481	−1.937	−2.303	−2.251
$\langle 13,10|E2|33,30\rangle$	−6.295	−3.240	−6.554	−6.128
$\langle 33,01|E2|33,21\rangle$	−3.942	−2.236	−3.854	−4.229
$\langle 33,21|E2|33,30\rangle$	4.122	3.742	4.152	4.350
$\langle 11,10|E2|11,10\rangle$	0.501	0.0	0.0	0.0
$\langle 11,10|E2|33,30\rangle$	0.649	0.0	0.0	0.0
$\langle 11,01|Ml|11,10\rangle$	−0.902	−1.155	−0.912	−0.949
$\langle 11,10|Ml|11,10\rangle$	1.560	1.633	1.585	1.621
$\langle 13,11|Ml|33,10\rangle$	−0.439	−0.646	−0.509	−0.531
$\langle 13,21|Ml|33,21\rangle$	−0.603	−0.646	−0.586	−0.641
$\langle 33,01|Ml|33,10\rangle$	−1.098	−1.291	−1.096	−1.061
$\langle 33,30|Ml|33,30\rangle$	3.122	3.055	3.106	3.032
$\langle 11,01|Ml|33,10\rangle$	−0.100	0.0	0.0	0.0
$\langle 11,01|Ms|11,10\rangle$	0.289	0.289	0.280	0.270
$\langle 11,10|Ms|11,10\rangle$	−0.336	−0.408	−0.360	−0.383
$\langle 11,10|Ms|13,20\rangle$	0.804	0.913	0.829	0.856
$\langle 11,10|Ms|13,21\rangle$	−0.819	−0.913	−0.839	−0.855
$\langle 33,01|Ms|33,10\rangle$	−0.618	−0.646	−0.620	−0.604
$\langle 33,30|Ms|33,30\rangle$	1.460	1.528	1.476	1.433
$\langle 11,01|Ms|33,10\rangle$	0.041	0.0	0.0	0.0

the orbital and spin parts of the $M1$ operator. The calculation is performed in the m scheme and subsequently transformed to the J,T basis. To get all the reduced matrix elements, full-space calculations with $M_J=0$ and $M_J=1$ must be done. In Table II we present selected matrix elements of pieces of Eq. (5), namely the operators

$$E2\equiv\sqrt{16\pi/5}\sum_{i=1}^{A}\left(\tfrac{1}{2}+t_{zi}\right)r_i^2Y^{(2)}(\Theta_i), \tag{6a}$$

$$Ml\equiv\sum_{i=1}^{A}\left(\tfrac{1}{2}+t_{zi}\right)\mathbf{l}_i, \tag{6b}$$

$$Ms\equiv\sum_{i=1}^{A}\left(\tfrac{1}{2}+t_{zi}\right)\mathbf{s}_i. \tag{6c}$$

These matrix elements are reduced in J and for $T_z=0$. The second column shows the matrix elements of the effective operators, as obtained from Eq. (4) and the procedure outlined above. Note that these operators, when used with the eigenvectors of the effective Hamiltonian obtained from Eq. (3), whose matrix elements are shown in Table I, give the same mean values and transition rates as the original one-body operators (6), when used with the $0\hbar\Omega$ dominated eigenvectors of the $6\hbar\Omega$ calculation. Also note that the effective operators are two-body operators unlike the full-space original operators.

TABLE III. Effective charges of the proton quadrupole, magnetic orbital, and magnetic spin operators, derived by least-square fits to the corresponding $0p$-shell effective operators obtained from the $6\hbar\Omega$ calculation for ^{6}Li. Both the j-dependent and j-independent effective charges are shown. Also, the j-independent effective charges obtained in the same way from the $4\hbar\Omega$ calculation are presented in the last two columns. For the definition of the effective charges see Eq. (7).

	$e^{p}_{(1/2\ 3/2)}$	$e^{n}_{(1/2\ 3/2)}$	$e^{p}_{(3/2\ 3/2)}$	$e^{n}_{(3/2\ 3/2)}$	$e^{p}_{(1/2\ 1/2)}$	$e^{n}_{(1/2\ 1/2)}$
$E2$	1.606	0.417	1.417	0.307	-	-
Ml	0.848	0.060	0.933	0.084	0.880	0.090
Ms	0.914	−0.006	0.963	0.003	0.925	−0.043
	$e^{p}_{\rm eff}$	$e^{n}_{\rm eff}$	$e^{p}_{\text{eff-4}}$	$e^{n}_{\text{eff-4}}$		
$E2$	1.527	0.364	1.302	0.244		
Ml	0.907	0.085	0.931	0.063		
Ms	0.937	0.001	0.953	−0.003		

Let us first discuss the $E2$ operator. In the third column of Table II the reduced matrix elements of the operators (6), evaluated in the P space, are shown for comparison. We observe, that there is a striking difference in the renormalization of the isoscalar and isovector matrix elements of $(E2)_{\rm eff}$. The former are much larger in magnitude than the latter in comparison with the unrenormalized values of the operator (6a). Apparently, there is no chance to approximate the effective operator as (6a) multiplied by some effective charge. Instead, it is possible to mimic the mentioned isoscalar-isovector effect by approximating the effective operator as a combination of one-body proton *and* neutron operators with different effective charges, e.g.,

$$(E2)_{\rm eff}\approx e^{p}_{\rm eff}\sqrt{16\pi/5}\sum_{i=1}^{A}\left(\tfrac{1}{2}+t_{zi}\right)r_i^2Y^{(2)}(\Theta_i) + e^{n}_{\rm eff}\sqrt{16\pi/5}\sum_{i=1}^{A}\left(\tfrac{1}{2}-t_{zi}\right)r_i^2Y^{(2)}(\Theta_i), \tag{7}$$

where only valence nucleons contribute in the sums. A better approximation may be obtained when the effective charges become j dependent, e.g., $\Sigma_{ij}e_{{\rm eff}ij}\langle i|\hat{O}|j\rangle a_i^{\dagger}a_j$ in the second-quantization form. We calculated the effective charges from the reduced matrix elements of the appropriate operators by a least-square fit. The resulting j dependent, as well as j independent, effective charges are presented in Table III, and the corresponding reduced matrix elements are shown in the fourth and fifth columns of Table II. First, we observe that this kind of approximation works very well. Moreover, the pure two-body matrix elements, which cannot be reproduced by an approximation of the type (7), are almost a factor of ten smaller than the largest one-body matrix elements. Second, the calculated effective charges $e^{\mathrm{p}}_{\mathrm{eff}}=1.527e$, $e^{\mathrm{n}}_{\mathrm{eff}}=0.364e$ are close to the phenomenological ones mentioned in the Introduction. Third, the j dependence of the effective charges is rather moderate.

From the phenomenological studies it is well known that the magnetic dipole transitions and moments can be in most cases described, at least in light nuclei, by using the operator (5b) with small modification of the g factors. Also the effective orbital and spin operators obtained in our study are much less renormalized, when compared to the starting one-body operators, than the electric quadrupole operator. It is reflected in the second and third parts of Table II. The isoscalar-isovector effect is much smaller, and, in the case of the spin operator it is almost nonexistent. Unlike the case of the quadrupole operator, the effective dipole operator matrix elements are, on average, smaller in comparison with one-body ones. A perhaps surprising result is, however, the observation that the orbital part is more renormalized than the spin part and, moreover, a neutron orbital part is generated with an effective g factor $g^{\mathrm{n}}_{l\mathrm{eff}}=0.085$. The proton g factor is about 10% quenched $g^{\mathrm{p}}_{l\mathrm{eff}}=0.907$. The spin part is quenched by about 6%, e.g., $g^{\mathrm{p}}_{s\mathrm{eff}}=0.937g^{\mathrm{p}}_s+0.001g^{\mathrm{n}}_s$ and from the isospin symmetry $g^{\mathrm{n}}_{s\mathrm{eff}}=0.937g^{\mathrm{n}}_s+0.001g^{\mathrm{p}}_s$. As in the quadrupole operator case, the j dependence is also moderate for the magnetic dipole operator effective charges, but the pure two-body matrix elements are relatively smaller.

The j-independent effective charges extracted in the same way from the $4\hbar\Omega$ calculation are also presented in Table III. We observe that the renormalization is smaller in this case. This reflects the fact that, for example, the $E2$ transition rates obtained in the $4\hbar\Omega$ calculation are weaker than those calculated in the $6\hbar\Omega$ space. Our observation here is that the effective Hamiltonian converges more rapidly than the $E2$ operator with respect to the full-space size change.

To quantify the two-body content of the effective $0p$-shell electromagnetic operators, we evaluate the quantity $R\equiv\sqrt{\Sigma_{i\leqslant j}(\hat{O}_{\mathrm{eff},ij}-\hat{O}_{\mathrm{ob\text{-}eff},ij})^2/\Sigma_{i\leqslant j}(\hat{O}_{\mathrm{eff},ij})^2}$, where the $\hat{O}_{ij}$ denotes the matrix elements between the $0p$-shell two-body states i and j. In this way we estimate the part of the effective operators, which cannot be expressed as a combination of one-body operators. When using one-body operators with j-dependent charges, we obtain a two-body contribution of 10.1% for $E2$, 3.8% for Ml, and 3.2% for Ms, respectively. For the one-body operator with j-independent effective charges the two-body contributions are 12.3% for $E2$, 5.3% for Ml, and 4.4% for Ms, respectively. Clearly, the magnetic dipole operators are better approximated by combinations of one-body operators.

In conclusion, we have shown that model-space truncation is sufficient to generate operator renormalization, which is characterized by effective charges compatible with those used in the phenomenological applications. We have found that the isoscalar and isovector parts of the operators are renormalized differently, particularly, in the case of the electric quadrupole operator. This difference in renormalization is the source of a nonzero neutron effective charge. These findings are based on a no-core $6\hbar\Omega$ calculation for ^{6}Li with a multivalued starting-energy-independent two-body interaction derived microscopically from the Reid 93 nucleon-nucleon potential, from which the $0\hbar\Omega$ $0p$-shell effective Hamiltonian, electric quadrupole, and magnetic dipole operators were constructed. The obtained effective operators are two-body operators. We have shown, however, that they may be well approximated by one-body operators. Their two-body content is about 10% for $E2$ and about 4% for $M1$ operators, respectively. We also studied the dependence of the renormalization on the size of the full space. We observed a non-negligible difference between the effective $E2$ charges extracted from the $6\hbar\Omega$ calculation in comparison to those obtained from the $4\hbar\Omega$ calculation. On the other hand, the changes in the effective Hamiltonians obtained in the two calculations are less pronounced.

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