Shell model calculation of the nuclear moments of ^{9}Li in a $2\hbar\omega$ space

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A recent measurement of the magnitude of quadrupole moment of the ground state of ^{9}Li, $Q(^9\text{Li})$, finds that $|Q(^9\text{Li})/Q(^7\text{Li})| = 0.88\pm0.18$. A variety of shell-model calculations, using p-shell wave functions, predict $Q(^9\text{Li}) \simeq 1.3Q(^7\text{Li})$ and yield quadrupole moments whose magnitudes are approximately half the experimental values. Agreement between theory and experiment is improved when effective charges are used, although the results are still not completely satisfactory. A calculation of the wave functions of the low-lying states of ^{7}Li and ^{9}Li using a modified version of the Sussex matrix elements in a model space, including all $0\hbar\omega$ and $2\hbar\omega$ excitations, has been performed. The resulting value for $Q(^9\text{Li})$ was -3.46 fm^2 as compared with the experimental value of $\pm3.22\pm0.66$ fm^2. The effective charge used in the calculation, $0.28e$, reproduced the experimental value of $Q(^7\text{Li})$ exactly. The calculated magnetic dipole moment of the ground state of ^{9}Li is 3.32 μ_N, the experimental value is ±3.44 μ_N.

I. INTRODUCTION

Recently measurements of the magnetic dipole and electric quadrupole moments of the ground state of ^{9}Li have been reported.[1] These measurements provide an interesting test of the various interactions proposed for use in the p shell. Comparisons quoted in Ref. 1 between experimental moments of ^{7}Li and ^{9}Li and those calculated using the wave functions of Cohen and Kurath[2] and those of Barker[3] lead to the following general conclusions; agreement between theory and experiment is satisfactory for the magnetic dipole moments, and agreement in the case of the electric quadrupole moments is much less satisfactory.

The large differences between experiment and theory in the case of the electric quadrupole moments are not unexpected. Shell-model calculations which do not include core excitations and limit configuration mixing will often severely underestimate electric quadrupole moments and transition rates. A wave function drawing on configurations from a single shell cannot approximate the collectivity which can lead to a large enhancement in the matrix elements of the $E2$ operator.

The standard approach to producing effective electric multipole operators, which are required by a truncated model space, has been the introduction of a neutron and proton effective charge. In general it is found that the $\Delta T=1$ isovector experimental $E2$ transition rates are reproduced when one takes $e_p - e_n = e$. This implies that an appropriate form for the effective charges is $e_p = e+\delta e$ and $e_n = \delta e$. Thus the isoscaler charge $e_p + e_n$ is increased by $2\delta e$ but the isovector charge is left at its bare nucleon value. The introduction of effective operators through the simple artifice of effective charges, as we will see below, produces a marked improvement in agreement between theory and experiment for ^{9}Li. However, it is found that a considerably smaller effective charge is required to fit the ground state quadrupole moment of ^{9}Li, at least when the Cohen and Kurath wave functions are used, than is generally required to fit the electric quadrupole properties of other p-shell nuclides. One would expect this state dependence of the effective charge to be significantly reduced if the shell-model calculation were carried out in a larger basis. It is primarily this point we wish to address in this paper.

This situation seemed to provide an interesting opportunity to test a modified version of the Sussex interaction proposed recently.[4] This interaction was used successfully in calculating, with no adjustable parameters, the binding energies of ^{3}He, ^{3}H, and ^{4}He in a shell-model basis including all excitations through $4\hbar\omega$. Thus, from energy considerations, it would be possible to do calculations on ^{9}Li with this interaction which included all excitations through $2\hbar\omega$. Therefore we are able to compare the results of our lowest order ($0\hbar\omega$) calculation with similar calculations and, more importantly, to gauge the effect of enlarging the basis space on the effective charge.

Unfortunately the test is not as definitive as it might be in that the experimental method may be subject to large systematic errors. The quantity actually measured in the experiment is the ratio of the quadrupole coupling of ^{9}Li to that of ^{7}Li in a $LiNbO_3$ crystal. It is assumed that the electric field gradient seen in the crystal by either isotope of Li is the same. Based on this assumption the ratio of the quadrupole coupling for the two isotopes is equal to the absolute value of the ratio of the quadrupole moments. It is the ratio of the ^{9}Li to the ^{7}Li ground-state quadrupole moments, $|Q(^9\text{Li})/Q(^7\text{Li})|$, which is deduced in the experiment. However, it is shown in Ref. 1 that the above assumption concerning the electric field gradients may introduce systematic errors of the order of 20% in this ratio. Therefore while the measurement of the quadrupole coupling is quite accurate the nature of the experiment is such that the quadrupole moment obtained is much less so.

II. METHOD OF CALCULATION

Our calculations of the ground-state wave functions of ^{7}Li and ^{9}Li were carried out in the m scheme where both a $0\hbar\omega$ space and one including all $0\hbar\omega$ and $2\hbar\omega$ excitations were used. The two-body matrix elements were constructed from the modified version of the Sussex relative matrix elements projected into a space of $4\hbar\omega$ maximum relative energy as described in Ref. 4. The size parameter used in these calculations was $b=1.6$ fm, the largest for which the modified matrix elements are available. The calculations also included the Coulomb potential and have spurious center of mass motion removed by the method of Palumbo.[5] No correction has been made to the electric quadrupole operator for center of mass motion.

For purposes of comparison calculations were carried out in a $0\hbar\omega$ space using the Cohen and Kurath[2] 6—16 2BME (two-body matrix elements) and the Hauge and Maripuu[6] effective p-shell interaction. In the case of the 6—16 2BME, the two-body matrix elements of the effective interaction and the single-particle energies are treated as parameters to be fit to selected states of the p-shell nuclei. The Hauge and Maripuu two-body matrix elements are based on the Sussex matrix elements[7] with $b=1.7$ fm, where the two-body matrix elements are modified through perturbation theory, including all $2\hbar\omega$ intermediate states, to produce an effective p-shell interaction. In their calculations the single-particle energies were treated as parameters used to fit the spectrum of each nucleus. In the results presented below, calculated using this effective interaction, the single-particle energies for ^{9}Be were used in the ^{9}Li calculations.

III. RESULTS AND DISCUSSION

The ground-state quadrupole moments calculated using wave functions derived from the various interactions discussed above are presented as a function of effective charge in Table I. The differences among the three calculations carried out in a $0\hbar\omega$ space are primarily due to the assumptions made concerning the mean-square radii. In the present work we used the modified Sussex matrix elements calculated for a harmonic oscillator size parameter, $b=1.6$ fm, while Hauge and Maripuu used those for $b=1.7$ fm. Hence the appropriate mean-square radii in a $0\hbar\omega$ calculation are 6.40 and 7.225 fm^2, respectively. For the Cohen and Kurath calculations the mean square radius used was 7.056 fm^2, the radius used in Ref. 1.

In Table II we present the effective charges which reproduce the experimental values of the ground-state quadrupole moments,[8,1] $Q(^7\text{Li})=-3.66\pm0.03$ fm^2 and $Q(^9\text{Li})=\pm3.22\pm0.66$ fm^2. In calculating the effective charges it was assumed that the negative sign was appropriate for $Q(^9\text{Li})$. In Table II it can be seen that the effective charges deduced from the $0\hbar\omega$ calculations for ^{7}Li have little or no overlap with those calculated for ^{9}Li. Furthermore, in most cases they are far from the accepted value for such calculations, $\delta=0.5$. On the other hand the effective charges deduced for the two isotopes from the $2\hbar\omega$ calculation using the modified Sussex matrix elements agree quite well. It must be noted that the effective charge is a state dependent quantity and therefore not necessarily the same for the two nuclei. However, one would expect the state dependence to be reduced as the basis size is expanded, and further, that the magnitude of the effective charge would decrease. Both these effects are seen in the present calculation.

As we mentioned above there is very little difference among the three quadrupole moments calculated in the $(Os)^4(Op)^{A-4}$ basis if one normalizes the results to the mean-square radius. This point is easily seen in Table III where we display the ratio of the shell-model calculation of $|Q(^9\text{Li})/Q(^7\text{Li})|$, as a function of the effective charge, to the experimental value, 0.88. Due to this normalization and the 20% uncertainty in the experiment, any value appearing in the table between 0.8 and 1.2 is in agreement with the experiment. This requirement is met in all three $0\hbar\omega$ calculations for effective charges of 0.4 or 0.5. Of the three calculations only the present one gives an acceptable ratio at a value of the effective charge which will also reproduce the ground state moment of ^{7}Li. Again we point out that this is primarily due to differences in the mean-square radii used in the calculation.

Again referring to Table III we see the ratio calculated using all excitations through $2\hbar\omega$ is a slowly varying function of the effective charge. Furthermore, the ratio is within the experimental limits for all reasonable values of the effective charge. At the value of the effective charge which best fits $Q(^7\text{Li})$, $0.28e$, one finds $Q(^9\text{Li})=-3.46$ fm^2 which agrees with experiment, assuming the negative experimental value is correct.

It would of course be interesting to investigate other electric quadrupole properties of these two nuclei. Unfortunately the only other such quantity known experimentally is the transition rate between the first excited state and the ground state of ^{7}Li. The results of our calculations for this transition along with the experimental value are presented in Table IV. The theoretical values were

TABLE I. Calculated ground-state quadrupole moments as a function of the effective charge, δe.

	$Q(^7\text{Li})$ (fm^2)	$Q(^9\text{Li})$ (fm^2)
Cohen and Kurath[a]	$-1.750-5.019\delta$	$-2.292-4.314\delta$
Hauge and Maripuu[b]	$-1.803-5.056\delta$	$-2.296-4.283\delta$
Present work ($0\hbar\omega$)	$-1.476-4.450\delta$	$-1.865-3.863\delta$
Present work ($2\hbar\omega$)	$-2.081-5.687\delta$	$-2.081-4.713\delta$

[a]Calculated using the 6—16 2BME tabulated in Ref. 2.
[b]Calculated using the two-body matrix elements tabulated in Ref. 6.

TABLE II. Effective charges which reproduce the experimental ground-state quadrupole moments of ^{7}Li and ^{9}Li.

	$\delta(^7\mathrm{Li})$	$\delta(^9\mathrm{Li})$
Cohen and Kurath[a]	0.381(7)	0.125(153)
Hauge and Maripuu[b]	0.367(7)	0.216(154)
Present work ($0\hbar\omega$)	0.491(7)	0.351(171)
Present work ($2\hbar\omega$)	0.278(6)	0.242(138)

[a]Calculated using the 6–16 2BME tabulated in Ref. 2.
[b]Calculated using the two-body matrix elements tabulated in Ref. 6.

calculated using the assumptions concerning the mean-square radii noted above and the effective charges which reproduced the experimental value of $Q(^7\mathrm{Li})$ (see Table II). It is clear that all the calculations are in agreement with each other and with experiment.

Although we wish to concentrate on the electric quadrupole properties, our confidence in the $2\hbar\omega$ ground-state wave function for a ^{9}Li is increased when we compare the calculated magnetic dipole moment, 3.32 μ_N, to the experimental value[1] of ± 3.44 μ_N and the $0\hbar\omega$ result of 3.04 μ_N. In addition, other calculations[9] of the properties of the p-shell nuclei using this interaction suggest that an effective charge of approximately $0.3e$ is appropriate for the quadrupole moments of nuclides in this region.

These calculations have been performed in the m scheme and hence in the n-p formalism. It is, however, possible to translate the results into the language of isospin. We find that the isoscaler contribution to Q increases in magnitude by about 30% in ^{7}Li and about 20% in ^{9}Li as the basis is enlarged. The small isovector contribution to Q, approximately 1% (4%) for ^{9}Li in $0\hbar\omega$ ($2\hbar\omega$), is opposite in phase to that of the isoscaler and is essentially unchanged in ^{7}Li while it quadruples in size in ^{9}Li. Thus the enhancement of both quadrupole moments is due only to the isoscaler contribution. The isoscaler contribution is also, of course, primarily responsible for the enhancement of $Q(^7\mathrm{Li})$ relative to $Q(^9\mathrm{Li})$. However, due to the opposing phase, the increase in the magnitude of the small isovector contributions provides a further reduction in the ratio of $Q(^9\mathrm{Li})$ to $Q(^7\mathrm{Li})$.

TABLE III. Ratio of the shell-model prediction for $|Q(^9\mathrm{Li})/Q(^7\mathrm{Li})|$, as a function of the effective charge, δe, to the experimental value for this quantity, 0.88.

	$\lvert Q(^9\mathrm{Li})/Q(^7\mathrm{Li})\rvert/0.88$			
δ	CK[a]	HM[b]	Present work ($0\hbar\omega$)	Present work ($2\hbar\omega$)
0.0	1.49	1.45	1.44	1.14
0.1	1.38	1.34	1.33	1.10
0.2	1.30	1.27	1.27	1.07
0.3	1.25	1.23	1.22	1.05
0.4	1.22	1.19	1.19	1.04
0.5	1.19	1.16	1.17	1.04

[a]Calculated using the 6–16 2BME presented in Ref. 2.
[b]Calculated using the two-body matrix elements presented in Ref. 6.

TABLE IV. $B(E2)$ for the $\frac{1}{2}^- \rightarrow \frac{3}{2}^-$ transition in ^{7}Li. The effective charge used in each case is that which reproduces the ground-state quadrupole moment exactly (see Table II).

		$B(E2)$ e^2 fm^4		
CK[a]	HM[b]	Present work ($0\hbar\omega$)	Present work ($2\hbar\omega$)	Expt.[c]
10.6	9.8	12.6	13.0	14(8)

[a]Calculated using the 6–16 2BME presented in Ref. 2.
[b]Calculated using the two-body matrix elements presented in Ref. 6.
[c]Reference 8.

Clearly it would be of interest to isolate those configurations represented in the ground-state wave functions which are the largest contributors to the enhancement of the quadrupole moments. As we have stated above, these calculations were performed in the m scheme. Thus, unfortunately this information cannot be extracted from the 1961 amplitudes in the ^{7}Li eigenvector and the 3958 amplitudes in the ^{9}Li without a considerable amount of additional calculation which we are currently not equipped to perform.

We have used a large basis space in these calculations in order to minimize the A dependence of the effective interaction and effective electromagnetic operators for a given size parameter. It is also of interest to see to what extent the results depend on the choice of size parameter. To this end we have repeated the calculations described above using the effective interaction for $b=1.5$ fm. We find that the results presented in the last two columns of Table III, which were calculated using $b=1.6$ fm, are reproduced essentially exactly in the 1.5 fm calculation. Furthermore, the effective charge which reproduces $Q(^7\mathrm{Li})$ in a $2\hbar\omega$ calculation, $\delta=0.34e$, gives -3.37 fm^2 for $Q(^9\mathrm{Li})$ and $12.8e^2$ fm^4 for the reduced transition rate between the first excited state and ground state of ^{7}Li. These results are in excellent agreement with those calculated using $b=1.6$ fm.

We have chosen to perform these calculations using a single model for ^{7}Li and ^{9}Li; that is, for purposes of comparison, we use a single size parameter, effective interaction, and effective charge. An alternate approach would be to use size parameters deduced from mean square radii of the two nuclei. However, the effective electromagnetic operators are a function of size parameter. Hence, one would require more experimental information concerning the electric quadrupole properties of ^{9}Li than is currently known to fix the effective charge. The calculations described above suggest that if this parameter were fixed by calculating the properties of other nuclei, one would find that the calculated $Q(^9\mathrm{Li})$ is insensitive to the choice of size parameter.

In summary, we have calculated the ground state wave functions of ^{7}Li and ^{9}Li in both a $0\hbar\omega$ and $2\hbar\omega$ space. The $0\hbar\omega$ wave functions, calculated using three different effective interactions, all predict $Q(^9\mathrm{Li})/Q(^7\mathrm{Li})\approx 1.1$ for reasonable values of the effective charge. The $2\hbar\omega$ wave functions calculated using both $b=1.6$ and 1.5 fm give $Q(^9\text{Li})/Q(^7\text{Li})\approx 0.9$ in agreement with experiment. This result emphasizes the well-known importance of configuration mixing in determining the electric quadrupole properties of nuclei. It is found that a single reasonable value of the effective charge, the only adjustable parameter in the calculation, provides good agreement between calculation and experiment for the two ground-state quadrupole moments and the reduced quadrupole transition rate between the first excited state and ground state of ^{7}Li. The calculated magnetic dipole moment of the ground state of ^{9}Li is in reasonable agreement with experiment.

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