In this preliminary survey of higher order corrections, particular attention has been paid to virtual $E2$ excitation, since the low-energy transitions in even-even nuclei undergoing collective excitations are known to be predominantly of the electric quadrupole type.[5] However, the possibility of virtual transitions of different multipolarity is not ruled out. Estimates[16] of a second $M1$ or $E4$ transition in the sequences $0^+(E2)2^+(M1)2^+$ and $0^+(E4)4^+(E2)2^+$ indicate that such effects are not expected to be serious in comparison to the $E2$ effects, at least in studies of the reorientation effect in even-even nuclei under conditions of low-energy heavy-ion bombardment. The possibility of second-order $E1$ transitions via the giant dipole resonance has been pointed out by Eichler[17] in connection with the reorientation effect in $Cd^{114}$. Recent estimates by MacDonald[18] indicate, however, that such effects may not be serious.


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# Quadrupole Deformation in $Li^7$†

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The quadrupole deformation of $Li^7$ is calculated by generating many-particle wave functions from deformed single-particle orbitals. In order to account for the $E2$ properties of $Li^7$ and retain the dominance of the basic shell-model configuration, excitation of the $(1s)^4$ core must be included. The admixtures of higher configurations are appreciable.

## I. INTRODUCTION

RECENT detailed calculations[1,2] of the electric-field gradients in LiH have led to an accurate value for the quadrupole moment of $Li^7$, namely $Q(Li^7) = -0.043$ b. van der Merwe showed[3] that this is much greater than one obtains with the usual $(1s)^4(1p)^3$ configuration. He showed that an effective charge of $\frac{1}{2}$ was needed to get the experimental result and also produce agreement with the measured $B(E2)$ strength[4] between the ground state and the first excited state. Recently, Present[5] reproduced the experimental value for $Q(Li^7)$ by mixing $^2P$ states from $(1p)^3$, $(1p)^2(2p)$, and $(1p)^2(1f)$—leaving the $(1s)^4$ core intact. The intensity found for the $(1p)^3$ component was only 35%.

The method of generator coordinates offers a direct procedure[6] for calculation of such configuration mixtures, starting from single-particle orbitals in a field of quadrupole deformation. It is also simple to include deformation of the $(1s)^4$ core with this method. Such an effect should certainly be included since the experimental value for $Q(Li^7)$ is about 1.8 times the value computed for $Q(Li^7)$ with the $(1s)^4(1p)^3$ configuration. As is seen from Present's results, such a large effect is difficult to obtain by deforming only the $1p$ orbitals. The objective of the calculation is to see whether one can account for the large quadrupole effects while keeping the $(1s)^4(1p)^3$ configuration dominant in $Li^7$.

## II. PROCEDURE

The application of the generating procedure to $Li^7$ is considerably simplified by the fact that the energy spectrum and magnetic-dipole properties are well described by a model with negligible spin-orbit coupling. It has been shown[3] that for $Li^7$ the inclusion of spin-orbit coupling within the $1p$ shell increases the quadrupole moment not more than 10% above its value at the Wigner supermultiplet limit

$$Q(Li^7, {}^2P[4+3]) = -(6/25)e\langle r^2\rangle_{1p,1p}. \quad (1)$$

Here $\langle r^2\rangle_{1p,1p}$, the expectation value of $r^2$ evaluated with $1p$ radial functions, has a magnitude $\langle r^2\rangle_{1p,1p} \approx 10^{-25}$ cm$^2$. Therefore the desired enhancement must come from outside the $1s$ and $1p$ shells, and thus is most

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simply computed in the limit in which spin-orbit coupling becomes negligible.

The starting point is the Nilsson diagram[7] in the asymptotic limit of large prolate deformation. The $Li^7$ generator is formed by putting two neutrons and two protons in the lowest level ($\Lambda=0^+$) and two neutrons and one proton in the next level ($\Lambda=0^-$). The quantity $\Lambda$ is the projection of orbital angular momentum (parity $\pm$) on the nuclear symmetry axis. The spatial wave function then has symmetry $S[4+3]$ as is clear in Eq. (4). The spin–isobaric-spin function with $S=\frac{1}{2}$, $T=\frac{1}{2}$ is just the function of complementary symmetry needed to give over-all antisymmetry when multiplied by the spatial function.

Therefore we can concentrate on the spatial function which is made from the single-particle spatial functions

$$\begin{aligned}\phi_0{}^+&=\phi_0{}^{1s}+\epsilon_{1d}\phi_0{}^{1d},\\ \phi_0{}^-&=\phi_0{}^{1p}+\epsilon_{2p}\phi_0{}^{2p}+\epsilon_{1f}\phi_0{}^{1f}.\end{aligned}\tag{2}$$

In Eq. (2) the single-particle functions are expanded in terms of spherical harmonic-oscillator functions $\phi^{nl}$. As described in Ref. 6 (hereafter called I) these functions contain contributions from shells having principal oscillator quantum numbers two units higher than those of the lowest order contribution. The admixture coefficients $\epsilon_i$ should be small and are given in first-order perturbation theory by

$$-\epsilon_i=\langle H_\delta\rangle_{0i}/2\hbar\omega.\tag{3}$$

The numerator is the matrix element of the quadrupole-deformation term in the Nilsson Hamiltonian. The spatial generating function, expanded in eigenfunctions of the total orbital angular momentum $L$, is

$$\chi_0=[\phi_0{}^+\phi_0{}^+\phi_0{}^+\phi_0{}^+][\phi_0{}^-\phi_0{}^-\phi_0{}^-]=\textstyle\sum_L C_L\Phi_0{}^L.\tag{4}$$

If $R$ is defined as the rotation that reverses the $y$ and $z$ axes, the application of $R$ to an eigenfunction $\phi_m{}^j$ of angular momentum $j$ and projection $m$ produces the result

$$R\phi_m{}^j=i^{2j}\phi_{-m}{}^j.\tag{5}$$

Applying $R$ to both sides of Eq. (4) using Eq. (2) shows that only odd $L$ occurs in the summation.

Following the procedure in I, the generator $\chi_0$ is expanded to terms linear in the $\epsilon_i$ by use of Eq. (2). The result is

$$\begin{aligned}\chi_0\approx&[(\phi^{1s})^4][(\phi^{1p})^3]+2\epsilon_{1d}[(\phi^{1s})^3\phi^{1d}][(\phi^{1p})^3]\\&+\sqrt{3}\epsilon_{2p}[(\phi^{1s})^4][(\phi^{1p})^2\phi^{2p}]\\&+\sqrt{3}\epsilon_{1f}[(\phi^{1s})^4][(\phi^{1p})^2\phi^{1f}].\end{aligned}\tag{6}$$

The magnetic quantum numbers have been suppressed in Eq. (6) because they are all zero. The wave functions are all normalized and have symmetry $S[4+3]$ as indicated by the square brackets. The states of interest in $Li^7$ have total angular momentum $J=\frac{1}{2}$ and $\frac{3}{2}$. Since the spatial generator of Eq. (6) contains only odd $L$, the $L=1$ component is the only one that can combine with the $S=\frac{1}{2}$ spin function to give a resultant $J=\frac{1}{2}$ or $\frac{3}{2}$. The terms of Eq. (6) can readily be expanded in eigenfunctions of $L$ by use of the raising and lowering operators $L^+$ and $L^-$. For example, if the $(1s)^4$ core is suppressed the term with coefficient $\epsilon_{2p}$ can be written

$$\begin{aligned}[\phi_0{}^{1p}\phi_0{}^{1p}\phi_0{}^{2p}]=&(\tfrac{3}{5})^{1/2}\Phi_0{}^P[(1p)^2 2p]\\&+(\tfrac{2}{5})^{1/2}\Phi_0{}^F[(1p)^2 2p],\end{aligned}\tag{6'}$$

where

$$\begin{aligned}(\sqrt{15})\Phi_0{}^P=&3[\phi_0{}^{1p}\phi_0{}^{1p}\phi_0{}^{2p}]-\sqrt{2}[\phi_0{}^{1p}\phi_{-1}{}^{1p}\phi_1{}^{2p}]\\&-\sqrt{2}[\phi_1{}^{1p}\phi_{-1}{}^{1p}\phi_0{}^{2p}]-\sqrt{2}[\phi_1{}^{1p}\phi_0{}^{1p}\phi_{-1}{}^{2p}].\end{aligned}\tag{7}$$

Each term on the right of Eq. (7) is a symmetric three-particle function indicated by the square bracket.

The complete wave function of the component of $\chi_0$ which has $L=1$, normalized to unity is

$$\begin{aligned}\Phi^P=N\{&\Phi^P[(1s)^4(1p)^3]+\sqrt{3}\epsilon_{2p}\Phi^P[(1s)^4(1p)^2 2p]\\&+(6/7)^{1/2}\epsilon_{1f}\Phi^P[(1s)^4(1p)^2 1f]\\&+(16/7)^{1/2}\epsilon_{1d}\Phi^P[(1s)^3 1d(1p)^3]\},\end{aligned}\tag{8}$$

where $N$ is just the normalization coefficient. The complete wave functions for the ground state and first excited state of $Li^7$ are obtained by vector coupling of $\Phi^P$ with the $S=\frac{1}{2}$ spin function to obtain a resultant of either $J=\frac{3}{2}$ or $J=\frac{1}{2}$.

## III. EVALUATION

From Eq. (3) one can show that the $\epsilon_i$ are proportional to matrix elements of the quadrupole operator $r^2Y_0{}^2$ evaluated between a lowest order single-particle wave function and a function from an oscillator shell with principal quantum number two units larger. Evaluation of $\langle r^2\rangle_{nl,n'l'}$ with harmonic-oscillator functions leads to the proportionality

$$\epsilon_{2p}:\epsilon_{1f}:\epsilon_{1d}::1:(27/8)^{1/2}:(15/8)^{1/2}.\tag{9}$$

The value of the quadrupole moment for $Li^7$, calculated with the wave function of Eq. (8), can be expressed in terms of $\epsilon\equiv\epsilon_{2p}$ through the relation

$$\begin{aligned}Q(Li^7)=&-(6/25)e\langle r^2\rangle_{1p,1p}\\&\times\left\{\frac{1+2(\sqrt{10})\epsilon+(90/7)\epsilon^2}{1+(285/28)\epsilon^2}\right\}.\end{aligned}\tag{10}$$

The bracket on the right of Eq. (10) is the enhancement factor $E$, since the quantity multiplying it is the value for the pure $1p$-shell configuration given in Eq. (1). The expression for $E$ is good only to terms quadratic in $\epsilon$ since higher order terms have been omitted. Values for the enhancement factor are listed in Table I, together with the amplitudes of the components in the wave function. There is a maximum value for $E$ which one can obtain from the expression in Eq. (10); this value is listed in the last row of Table I. For smaller values of $E$

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TABLE I. Results of the calculation when the enhancement factor $E$ has the values in column 1. The admixture coefficients $\epsilon_i$ of Eq. (2) are listed in columns 2–4. The amplitudes of the components of the ground-state wave function of Eq. (8) are listed in columns 5–8.

| $E$ | $\epsilon \equiv \epsilon_{2p}$ | $\epsilon_{1f}$ | $\epsilon_{1d}$ | $\alpha_0$ | $\alpha_{2p}$ | $\alpha_{1f}$ | $\alpha_{1d}$ |
|---|---|---|---|---|---|---|---|
| 1.50 | 0.082 | 0.150 | 0.112 | 0.968 | 0.136 | 0.135 | 0.164 |
| 1.79 | 0.142 | 0.261 | 0.194 | 0.910 | 0.224 | 0.220 | 0.268 |
| 2.00 | 0.211 | 0.387 | 0.289 | 0.830 | 0.303 | 0.298 | 0.362 |
| 2.13 (max) | 0.358 | 0.657 | 0.490 | 0.659 | 0.408 | 0.401 | 0.488 |

there are always two solutions for $\epsilon$ but only the smaller value is consistent with the assumption of small $\epsilon$ used in deriving Eq. (10).

If the value computed for the quadrupole moment at the Wigner supermultiplet limit is taken to be $-0.024$ b, the observed value of $-0.043$ b is obtained with an enhancement factor of $E=1.79$. For such a value one sees from Table I that the $(1s)^4(1p)^3$ configuration is still dominant in the wave function. However, the admixtures required to obtain this $E$ are appreciable.

Table II contains the matrix of the electric quadrupole moment in the space of the wave functions that make up Eq. (8). The last row of Table I is very nearly that corresponding to the largest negative eigenvalue of the matrix in Table II. However, it is also clear from Table I that near this extreme value there are wave functions that have appreciably different composition but give nearly as large a magnitude for the quadrupole moment. Such great sensitivity makes it difficult to deduce the composition of the wave function just from the observed quadrupole moment.

TABLE II. Matrix of the electric quadrupole moment of $Li^7$ in the space of the component wave functions that make up Eq. (8). All are $P_{3/2}[4+3]$ states, and the matrix is given in units of $(1/25)e\langle r^2\rangle_{1p,1p}$.

| | $\Phi_0$ | $\Phi_{2p}$ | $\Phi_{1f}$ | $\Phi_{1d}$ |
|---|---|---|---|---|
| $\Phi_0$ | $-6$ | $-(\frac{2}{5})(30)^{1/2}$ | $-(\frac{2}{5})(70)^{1/2}$ | $-(21)^{1/2}$ |
| $\Phi_{2p}$ | $-(\frac{2}{5})(30)^{1/2}$ | $-(38/5)$ | $-(8/15)(21)^{1/2}$ | 0 |
| $\Phi_{1f}$ | $-(\frac{2}{5})(70)^{1/2}$ | $-(8/15)(21)^{1/2}$ | $-(46/15)$ | 0 |
| $\Phi_{1d}$ | $-(21)^{1/2}$ | 0 | 0 | $-(29/4)$ |

If one does not include deformation of the $(1s)^4$ core, the enhancement factor becomes

$$E'=\left\{\frac{1+(\sqrt{10})\epsilon+(215/28)\epsilon^2}{1+(165/28)\epsilon^2}\right\}. \qquad (11)$$

This expression attains a maximum value of $E'=1.82$ for $\epsilon=0.52$. Since the experimental quadrupole moment indicates $E\approx 1.8$, a model with no $(1s)^4$ deformation is being pushed to its limit to fit experiment. This result is very close to that of Present[5] who obtained an enhancement $E'=1.86$ by diagonalizing the matrix of the quadrupole operator in a representation of $^2P[4+3]$ functions allowing no excitation of the $(1s)^4$ core. The resultant wave function for the ground state of $Li^7$ is also similar to that of Present since for $E'=1.82$ the intensity of the $(1p)^3$ configuration is only 38%. However, very large values for $\epsilon_{2p}$ and $\epsilon_{1f}$ are required to fit the experimental result if one does not deform the $(1s)^4$ core. This would imply that configurations with two nucleons excited into the $(2p,1f)$ levels are also important and would destroy the validity of the shell model for nuclei in this region.

## IV. CONCLUSIONS

The main conclusion of this calculation is that the generating procedure permits one to construct a shell-model picture which accounts for the observed quadrupole moment of $Li^7$ while still retaining the $(1s)^4(1p)^3$ configuration as the dominant one. Such a procedure requires including excitations from the $(1s)^4$ core in order that the out-of-shell admixtures are not unreasonable. Consistency between the quadrupole moment and the $B(E2)$ strength between the first two states of $Li^7$ is automatically ensured in this model since, as shown by Elliott[8] the relationship between these two quantities is the same as in the usual collective model.

The effect of going away from the limit of negligible spin-orbit coupling will give a slightly larger quadrupole moment. This effect can compensate to some extent for the neglect of the center-of-mass contribution in this calculation.

The results in Table I indicate that appreciable admixture coefficients are required to reproduce the experimental $E2$ properties of $Li^7$. The magnitude of these admixtures is notable especially since the method of obtaining them is designed to produce large $E2$ effects with a minimum of admixture. The amplitude of about 0.9 for the basic configuration is large enough to ensure that properties such as energies and $M1$ strengths are determined by the basic configuration. However, the several other components, each with 5–10% intensity are quite important, and should affect other properties such as form factors in electron scattering.

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