Li^7 Quadrupole Moment. II*

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(Received 29 January 1965)

The recently determined electric quadrupole moment Q of the Li^7 nucleus disagrees with the predictions of current nuclear models. It is shown that the quadrupole and magnetic moments, together with the Gamow-Teller matrix element for the $Be^7 \rightarrow Li^7$ (ground state) K capture, can be accounted for on the supermultiplet theory if the *ad hoc* wave function has a 65% admixture of the ^2P [3] states arising from the $1s^4 1p^2 2p$ (two) and $1s^4 1p^2 1f$ (one) configurations. Assuming equal configuration admixtures in both levels of the ground doublet term ($^2P_{1/2,3/2}$), the $M1$ and $E2$ transition strengths for quantum jumps between the ground state ($^2P_{3/2}$) and the first excited state ($^2P_{1/2}$) at 478 keV have been calculated and found to agree with measured values of B ($M1$) and B ($E2$) within experimental error. The reduced $E2$ transition strength in emission is given by: $B(E2) \cong Q^2$. Pure LS coupling and exact partition symmetry are assumed. The proportion of the ground configuration can be substantially increased by including the $1s^3 1p^3 1d$ configuration in the mixture.

I. MOLECULAR CALCULATIONS

MEASUREMENTS[1] of the nuclear quadrupole coupling constant eqQ in Li_2 failed to yield a value for the electric quadrupole moment Q of the Li^7 nucleus because the electric field gradient q in this molecule could not be accurately determined.[2] Whereas the electronic contribution to q is nearly cancelled by the contribution from the other nucleus in Li_2, a comparable cancellation is not expected in LiH and this circumstance, together with the greater accuracy attainable in the molecular four-electron problem, indicated that $Q(Li^7)$ might be successfully determined from quadrupole coupling measurements in LiH. These measurements have been made by Wharton, Gold, and Klemperer[3] and values of q in LiH have been calculated independently by Kahalas and Nesbet[4] and by Browne and Matsen.[5] The latter calculation provides the best wave function so far obtained for this molecule (the total energy is within 0.176% of the experimental value and the wave function provides for polarization of the $1s$ shell). The values of q at both nuclei were calculated by Browne and Matsen and the q value at the hydrogen nucleus, when combined with the deuteron Q, reproduced the deuteron coupling constant in LiD within experimental accuracy.

The values of q at the Li nucleus obtained from the two molecular calculations with essentially different wave functions agree closely and indicate that $Q(Li^7) \cong -0.043$ barn. Current nuclear models predict a negative moment Q but the predicted magnitudes are about half of the observed value. The molecular calculations have not included a correction for the Sternheimer shielding effect[6] (due to the quadrupole moment induced in the Li $1s$ shell by the nuclear Q). A calculation[7] of this effect for the Li_2 molecule with different molecular wave functions indicates a reduction in the magnitude of q (by as much as 25%) unless there are fortuitous cancellations. Although no explicit calculation has been made, the shielding effect in LiH is expected to enhance the disagreement with the nuclear models.

II. NUCLEAR MODELS

$Q(Li^7)$ has previously been calculated from five nuclear models: (1) the Wigner supermultiplet theory (LS coupling),[8] (2) the simple jj-coupling model,[9] (3) the isospin jj-coupling model,[10] (4) the quasiatomic central-force model,[11] (5) the central- and tensor-force Hamiltonian,[12] and (6) the Inglis-Kurath central- and spin-orbit force Hamiltonian.[13] The first three models require no explicit representation of the Hamiltonian operator and no energy calculations need be made; the wave function (except for its radial part) is completely and uniquely determined in the case of Li^7 by the coupling scheme, quantum numbers, and symmetries. The last three models involve Hamiltonian calculations; models (5) and (6) refer to intermediate coupling schemes. Model (2), which is inconsistent with charge independence, and model (4), which gives substantially the same results as model (1), will not be considered further.

Table I compares predictions of the supermultiplet

* Supported in part by a grant from the National Science Foundation.

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[2] E. G. Harris, Ph.D. thesis, University of Tennessee, 1953 (unpublished); E. G. Harris and M. A. Melkanoff, Phys. Rev. **90**, 585 (1953).
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[4] S. L. Kahalas and R. K. Nesbet, J. Chem. Phys. **39**, 529 (1963).
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[7] R. M. Sternheimer and H. M. Foley, Phys. Rev. **92**, 1460 (1953).
[8] R. D. Present, Phys. Rev. **80**, 43 (1950).
[9] M. G. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure* (John Wiley & Sons, Inc., New York, 1955), p. 106.
[10] (a) B. H. Flowers, Phil. Mag. **43**, 1330 (1952); (b) E. Feenberg, *Shell Theory of the Nucleus* (Princeton University Press, Princeton, New Jersey, 1955), p. 145.
[11] S. Welles, Phys. Rev. **62**, 197 (1942).
[12] A. M. Feingold, Ph.D. thesis, Princeton University, 1952 (unpublished); Phys. Rev. **101**, 258 (1956).
[13] (a) D. Kurath, Phys. Rev. **101**, 216 (1956); (b) J. H. van der Merwe, Phys. Rev. **131**, 2181 (1963).

TABLE I. Ground-state properties of Li^7.

	Magnetic moment (in nm)	Quadrupole moment (in b)	Gamow-Teller matrix element: $\lvert\int\sigma\rvert^2$
Experimental value	3.256	-0.043	1.60 ± 0.15
Supermultiplet theory (LS coupling)	3.13	$-(6/25)\langle r^2\rangle_{1p}$ $\cong-0.024$	$5/3\cong1.67$
Isospin jj-coupling model ($T=\frac{1}{2}$)	3.04	$-(22/75)\langle r^2\rangle_{1p}$ $\cong-0.029$	$121/135\cong0.90$

theory and the isospin jj-coupling model with experimental results for the magnetic moment and quadrupole moment of Li^7 and the Gamow-Teller matrix element for the $Be^7\rightarrow Li^7$ (ground state) K capture. The magnetic moments agree with experiment within estimated exchange-current uncertainties. The predicted quadrupole moments are in terms of $\langle r^2\rangle_{1p}$, the mean-square radius of the $1p$ shell, which is determined empirically. From electron-scattering data[14] we estimate that $\langle r^2\rangle_{1p}\approx0.10$ b; this value is to be compared with $R^2\approx0.08$ b, where R is the Coulomb-energy radius. The predicted quadrupole moments are in significant disagreement with experiment. The LS coupling value[15] of the Gamow-Teller matrix element agrees well with the recently improved ft value[16]; the jj-coupling result[17] does not.

Nearly the same values of Q are obtained from the intermediate-coupling calculations. Feingold[12] was able to explain the inverted doublet structure of the two lowest levels of Li^7 in terms of the tensor interaction; he included higher configurations mixed in by the tensor force. The value of Q that corresponds to the experimental doublet spacing is about -0.017 b. Using Kurath's results, van der Merwe[13] estimated that $Q\approx-0.25\langle r^2\rangle_{1p}$. Thus the calculated values of Q are nearly independent of the coupling scheme.

III. SUPERMULTIPLET THEORY WITH CONFIGURATION MIXING

In a previous note[8] we attempted to account for a possible positive value[1] of $Q(Li^7)$ on the basis of the supermultiplet theory with configuration interaction. Of the configurations that interact with $1s^41p^3$, the lowest in energy are $1s^41p^22p$, $1s^41p^21f$, $1s^31p^31d$, $1s^31p^32s$, $1s^21p^5$, $1s^41p2s^2$, $1s^41p1d^2$, and $1s^41p2s1d$, and in the case of the isotropic oscillator potential they have all the same zero-order energy. The last five of these configurations are not connected with the ground state through the one-particle quadrupole-moment operator. The ground state ($1s^41p^3\,{}^2{}^2P_{3/2}$) has an orbital wave function, belonging to the partition [3], which is symmetric in the space coordinates of the three nucleons outside the s shell. Assuming that partition symmetry and LS coupling were both preserved, we obtained the ^2P functions of symmetry [3] arising from the $1s^41p^22p$ and $1s^41p^21f$ configurations (two $^2P[3]$ functions from the former and one from the latter). The matrix elements of Q were calculated and the radial integrals were expressed in terms of $\langle r^2\rangle_{1p}$ with the aid of oscillator eigenfunctions. The symmetric wave functions are listed in Table I and the corresponding matrix elements of Q in Table II of Ref. 8.

In view of the new experimental results we have reexamined the 4×4 matrix for Q to see if it would account for a large negative value of the quadrupole moment. The lowest eigenvalue of the Q matrix, corresponding to the largest negative Q obtainable from this admixture, is $-0.4456\ \langle r^2\rangle_{1p}\approx-0.045$ b. This is very close to the experimental value. The corresponding coefficients of the normalized eigenfunction (in the order of Tables I and II of Ref. 8) are 0.5893, -0.4297, 0.2790, and 0.6427; thus the basic configuration $1s^41p^3$ constitutes only 35% of the mixture. The admixture of $^2P[3]$ states from excited configurations has no effect on the magnetic moment nor on the Gamow-Teller matrix element, both of which are determined solely by the coupling scheme and the quantum numbers.[8]

Insofar as the quasi-atomic Hartree approximation is a poor one, a large amount of configuration mixing is to be expected. Furthermore, as stressed by Wigner, the assumption of a charge-independent, spin-independent Hamiltonian with exchange forces leads to a wide spread of the terms of different symmetry arising from a given configuration and therefore to significant overlapping of neighboring configurations (since the terms of greatest space symmetry of the upper configuration may be depressed below the least symmetric terms of the lower configuration). These two sources of configuration interaction are more important than the small mixing ($\sim5\%$) induced by the tensor force.[12] Few quantitative estimates of these effects are available: They have been studied, especially, by Margenau and his students[18] who, using central, exchange potentials of Gaussian form and harmonic-oscillator eigenfunctions, calculated the ground-state energies of light nuclei in higher approximations of the Hartree method. In the case of Li^7, the first approximation gave a binding energy of 12 MeV, but this was increased to 29 MeV when higher configurations were included. The $1s^41p^22p$ and $1s^41p^21f$ configurations contributed little to the second-order energy.

We have also investigated the effect of including the $^2D[3]$ states from the $1s^41p^22p$ and $1s^41p^21f$ configurations (the $1s^41p^3$ configuration gives rise to no D state of symmetry [3]). These two states are of negligible use in lowering the value of Q but they do impair

[14] R. Hofstadter, Rev. Mod. Phys. **28**, 214 (1956).
[15] E. Wigner, Phys. Rev. **56**, 519 (1939).
[16] J. N. Bahcall, Phys. Rev. **128**, 1297 (1962).
[17] A. Winther and O. Kofoed-Hansen, Kgl. Danske Videnskab. Selskab, Mat. Fys. Medd. **27**, No. 14 (1953) and Ref. 10(b), p. 138.
[18] W. A. Tyrrell, K. G. Carroll, and H. Margenau, Phys. Rev. **55**, 790 (1939); K. G. Carroll, Phys. Rev. **57**, 791 (1940).

the agreement with the magnetic moment. The inclusion of $^2P[3]$ states from other configurations could lead to a wave function yielding the experimental value of Q but containing a larger proportion of the ground configuration than 35%; this possibility has not yet been investigated.

IV. APPLICATION TO $M1$ AND $E2$ TRANSITIONS

The first excited state of Li^7, at 478 keV above the ground state, is the upper level ($^2P_{1/2}$) of the doublet P ground term in LS coupling. The mean lifetime of this state has been measured in resonance scattering and self-absorption experiments.[19] The transition to the ground state is nearly pure $M1$ and the mean lifetime of $(1.20\pm0.1)\times10^{-13}$ sec corresponds to a reduced transition strength for magnetic dipole radiation $B(M1)=18.2\pm2$, where

$$B(M1)\equiv|(J_i||\mathfrak{y}||J_f)|^2 = (2J_i+1)^{-1}\sum_{M_i}\sum_{M_f}|(J_iM_i|\mathfrak{y}|J_fM_f)|^2 \quad (1)$$

and $\mathfrak{y}$ is in nuclear magnetons. The reduced transition strength for the very weak $E2$ transition between the same two states has been measured by the method of Coulomb excitation.[20] Referring the result to the upper level, the reduced transition strength for electric quadrupole emission is given by $B(E2)=(15\pm3)\times10^{-52}$ cm^4, where

$$B(E2)\equiv|(J_i||\mathbf{Q}_2||J_f)|^2 = (2J_i+1)^{-1}\sum_{M_i}\sum_{M_f}|(J_iM_i|Q_2{}^{M_i-M_f}|J_fM_f)|^2$$

and (2)

$$Q_2{}^m=\sum_{i=1}^{Z} r_i{}^2Y_2{}^m(\theta_i,\phi_i) \quad \text{(over protons)}\,.$$

The double-bar expressions in Eqs. (1) and (2) are the reduced matrix elements defined by the Wigner-Eckart theorem. Using this theorem

$$B(E2)=\left[\frac{(J_iM_i|Q_2{}^0|J_fM_i)}{(J_f2M_i0|J_f2J_iM_i)}\right]^2. \quad (3)$$

We first consider these transitions on the assumption that the upper and lower levels are $^2P_{1/2}[3]$ and $^2P_{3/2}[3]$ states from the single configuration $1s^41p^3$. An elementary calculation shows that

$$B(M1)=3|(\tfrac{1}{2}\tfrac{1}{2}|\mu_z|\tfrac{3}{2}\tfrac{1}{2})|^2 = \tfrac{2}{3}(2\mu_P-\tfrac{1}{3})^2=18.4 \quad (4)$$

in close agreement with experiment. From Eq. (3) one has

$$B(E2)=5|(\tfrac{1}{2}\tfrac{1}{2}|Q_2{}^0|\tfrac{3}{2}\tfrac{1}{2})|^2 \quad (5)$$

and, in terms of the symmetry [3] orbital function $\Phi(P^i)$ for the $1p^3$ configuration,

$$(\tfrac{1}{2}\tfrac{1}{2}|Q_2{}^0|\tfrac{3}{2}\tfrac{1}{2})=(2^{1/2}/3) \times\left[\int Q_2{}^0|\Phi(P^1)|^2-\int Q_2{}^0|\Phi(P^0)|^2\right] = 2^{1/2}\int Q_2{}^0|\Phi(P^1)|^2 \quad (6)$$

with the aid of the Wigner-Eckart theorem. The integral in Eq. (6) was obtained in evaluating the static quadrupole moment. Finally,

$$B(E2)=(9/50\pi)(\langle r^2\rangle_{1p})^2 \approx 5.7\times10^{-52}\ \text{cm}^4 \quad (7)$$

using $\langle r^2\rangle_{1p}\approx0.10$ b. This result, which has already been obtained by van der Merwe[13b] is much smaller than the experimental value.

The effects of configuration mixing will now be examined. We neglect the small mixing induced by the tensor or spin-orbit forces and consider only the larger mixing caused by the central forces. In the absence of tensor and spin-orbit forces the two states of the doublet are degenerate and are equally perturbed by configuration interaction, the admixtures being the same in both states. Spin-orbit and tensor forces perturb the two states unequally and different admixtures of different states occur in the two wave functions. We assume that, to a good approximation, the configuration mixing is the same in the upper and lower states with the same coefficients. The wave functions of the two states are written as $\sum b_i\Psi_i(J=\frac{1}{2}, M=\frac{1}{2})$ and $\sum a_f\times\Psi_f(J=\frac{3}{2}, M=\frac{1}{2})$, the sums being over the same set of configurations and including $^2P[3]$ states only, and we shall ultimately set $b_i=a_i$. Then Eq. (4) is replaced by

$$(\tfrac{1}{2}\tfrac{1}{2}|\mu_z|\tfrac{3}{2}\tfrac{1}{2})=\sum_i\sum_f b_i{}^*a_fM_{if},$$

$$M_{if}=\sum_{\text{spin}}\int\Psi_i{}^*(J=\tfrac{1}{2}, M=\tfrac{1}{2})\mu_z\Psi_f(J=\tfrac{3}{2}, M=\tfrac{1}{2})\,. \quad (8)$$

All nondiagonal matrix elements M_{if} vanish. The nondiagonal terms in the spin part of the moment vanish through orthogonality of the space functions and the diagonal terms are all the same because all states have the same quantum numbers. The terms in the orbital part of the moment are given by

$$M_{if}{}^{(\text{orb})}=(2^{1/2}/3)\left[\int\Phi_i{}^*(P^1)l_{1z}\Phi_f(P^1) - \int\Phi_i{}^*(P^0)l_{1z}\Phi_f(P^0)\right]. \quad (9)$$

[19] C. P. Swann, V. K. Rasmussen, and F. R. Metzger, Phys. Rev. **114**, 862 (1959); W. L. Mouton, J. P. F. Sellschop, and R. J. Keddy, Phys. Rev. **128**, 2745 (1962).

[20] P. H. Stelson and F. K. McGowan, Nucl. Phys. **16**, 92 (1960); R. C. Ritter, P. H. Stelson, F. K. McGowan, and R. L. Robinson, Phys. Rev. **128**, 2320 (1962).

Since the orbital functions Φ_i and Φ_f are symmetric functions of the 1, 2, 3 space coordinates and form an orthonormal set

$$\int \Phi_i^* l_{1z} \Phi_f = \frac{1}{3} \int \Phi_i^* L_z \Phi_f = \tfrac{1}{3} M_L \delta_{if}. \tag{10}$$

Thus $M_{if}^{(\mathrm{orb})} = 0$ for $i \neq f$ and $M_{ii}^{(\mathrm{orb})} = 2^{1/2}/9$ for all diagonal elements. Since $M_{ii}^{(\mathrm{spin})} = -2^{3/2}\mu_P/3$ the result is

$$(\tfrac{1}{2}\tfrac{1}{2}|\mu_z|\tfrac{3}{2}\tfrac{1}{2}) = (2^{1/2}/3)(\tfrac{1}{3} - 2\mu_P) \sum b_i^* a_i \tag{11}$$

and with equal configuration admixtures in the two states ($b_i = a_i$), it follows that the $M1$ transition strength is unchanged from the single-configuration result (Eq. 4).

With configuration mixing Eq. (6) is replaced by

$$(\tfrac{1}{2}\tfrac{1}{2}|Q_2^0|\tfrac{3}{2}\tfrac{1}{2}) = \sum_i \sum_f b_i^* a_f Q_{if},$$

where

$$\begin{aligned} Q_{if} &= \sum_{\text{spin}} \int \Psi_i^*(J=\tfrac{1}{2}, M=\tfrac{1}{2}) Q_2^0 \Psi_f(J=\tfrac{3}{2}, M=\tfrac{1}{2}) \\ &= (2^{1/2}/3)\left[\int \Phi_i^*(P^1) Q_2^0 \Phi_f(P^1) - \int \Phi_i^*(P^0) Q_2^0 \Phi_f(P^0)\right] \\ &= 2^{1/2} \int \Phi_i^*(P^1) Q_2^0 \Phi_f(P^1) \end{aligned} \tag{12}$$

again using the Wigner-Eckart theorem. The static quadrupole moment Q of the ground state is given by

$$Q = \sum_i \sum_f a_i^* a_f \int \Phi_i^*(P^1)(16\pi/5)^{1/2} Q_2^0 \Phi_f(P^1). \tag{13}$$

Hence, if $b_i = a_i$,

$$(\tfrac{1}{2}\tfrac{1}{2}|Q_2^0|\tfrac{3}{2}\tfrac{1}{2}) = (5/8\pi)^{1/2} Q$$

and

$$B(E2) = 25Q^2/8\pi \cong Q^2. \tag{14}$$

This relation between $B(E2)$ and Q^2 is *independent of the configuration admixture* and it holds under the assumptions of LS coupling (only ^2P states included) and equal admixtures in the upper and lower states. Insertion of the experimental value of $Q \cong -0.043$ b into Eq. (14) gives $B(E2) \cong 18.4 \times 10^{-52}$ cm^4, which agrees with the Coulomb excitation measurement within the errors of both determinations. It is of interest, although of uncertain quantitative significance, that the collective model also predicts a relation between $B(E2)$ and Q^2 equivalent to Eq. (14).[13b,21]

[21] C. M. Chesterfield and B. M. Spicer, Nucl. Phys. **41**, 675 (1963). From the collective rotational model, these authors estimate that $Q = -0.029$ b.

Independent-particle wave functions of the type used here fail to provide for the uniform translation of the center of mass and two related consequences of this error are (a) the appearance of spurious states, and (b) a necessary modification of the matrix elements of the electromagnetic moments to take account of recoil effects.[22] In the case of oscillator wave functions, both of these effects have been shown to vanish for states in which there is no more than one incomplete shell. Thus, while the results obtained here for the basic $1s^4 1p^3$ configuration require no modification, the wave functions and electromagnetic-moment matrix elements for the $1s^4 1p^2 2p$ and $1s^4 1p^2 1f$ states require correction for spurious states and recoil effects. These corrections for the admixed states will not seriously alter the results and Eq. (14) will be unaffected.

In conclusion, it appears that the supermultiplet theory with configuration mixing provides a wave function that is consistent with the magnetic moment and electric quadrupole moment of the ground state, with the ft value for the $Be^7 \rightarrow Li^7$ (ground-state) K-capture, and with both the $M1$ and $E2$ transition strengths for quantum jumps between the ground state and the first excited level at 478 keV. No explicit representation of the Hamiltonian operator has been used and, of course, no energy calculation has been made. It is planned to extend these calculations to include configurations in which the α core is excited; the configuration $1s^3 1p^3 1d$ has been shown by Carroll[18] to make a greater contribution to the second-order energy than all other low excited configurations and it should also contribute significantly to the quadrupole deformation.[23] In contrast to the point of view of the collective model, the calculations of this paper demonstrate that a solution to the problem exists, consistent with the experimental data, in which the α core is *not* deformed.

Note added in proof. The symmetrized 7-nucleon wave function for the $1s^3 1p^3 1d\ ^2P$ state has been obtained and the matrix elements of Q calculated with the assistance of B. M. Morris. We check the result obtained by Dr. Kurath with generator coordinates.[23] The phases of the $1s^4 1p^2 1f$ and $1s^3 1p^3 1d$ functions are opposite to those of the $1s^4 1p^3$ and $1s^4 1p^2 2p^\times$ functions; the other $1s^4 1p^2 2p$ state was not used.

[22] J. P. Elliott and T. H. R. Skyrme, Proc. Roy. Soc. (London) **A232**, 561 (1955); S. Gartenhaus and C. Schwartz, Phys. Rev. **108**, 482 (1957); H. J. Lipkin, Phys. Rev. **110**, 1395 (1958).

[23] Dr. D. Kurath (after reading this paper in manuscript) estimated the effect of including the $1s^3 1p^3 1d$ configuration by the shorthand method of generator coordinates with the generator functions chosen to be complete single-particle states in a deformed well [cf., D. Kurath, Nucl. Phys. **14**, 398 (1960)]. His result is that "a value of $-0.43\ \langle r^2\rangle_{1p}$ can be obtained for the quadrupole moment with a wave function which has an amplitude of 0.91 for the $1s^4 1p^3$ configuration [the other amplitudes were: 0.268 ($1s^3 1p^3 1d$), 0.224 ($1s^4 1p^2 2p$), and 0.220 ($1s^4 1p^2 1f$)]." This result suggests that the Hartree approximation may be quite good in Li^7. The $1s^4 1p^3$ amplitude of 0.59, found in Sec. III, implies that the Hartree approximation is very poor. Both pictures are consistent with the experimental data for Li^7.