Triaxial Shapes for *sd*-Shell Nuclei*

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(Received 29 October 1971)

The $E2$ properties and excitation energies of low-lying states in ^{24}Mg, ^{26}Mg, ^{30}Si, and ^{32}S are calculated using the adiabatic model of a triaxially deformed rotor. The results are compared with those of recent shell-model calculations and strong similarity is found for both ^{24}Mg and ^{32}S with nearly the same deformation parameters in the adiabatic model. The strength for isovector $M1$ excitation, pertinent to results of inelastic electron scattering, is also calculated using the closure sum rule.

1. INTRODUCTION

Shell-model calculations have been carried out[1,2] for up to six particles (or holes) in the complete $2s1d$ space. For more particles one must truncate the space in order to have a feasible calculation.[3,4] The results of these calculations agree quite well with experimental observation.

The authors of Ref. 1 point out that for $A=18$–22 the excitation energies and $E2$ properties for low-lying states are quite similar to those of the rotational bands arising from an adiabatic rotational model. In this model, the quadrupole properties are obtained from an intrinsic state with particles in the lowest energy levels of an axially symmetric prolate deformed potential well (the Nilsson model). It is also well known that this model can be successfully applied to represent observations in nuclei with $A=23$–25.

Even-even nuclei in the central part of the $2s$-$1d$ shell exhibit level schemes that deviate from what is expected for an axially symmetric rotor. For ^{26}Mg and heavier nuclei, other states intrude in the low-excitation region. The common appearance of three additional states with angular momentum $I^\pi = 2^+$, 3^+, and 4^+ can be interpreted as the effect of departure from axial symmetry in the deformed field. The purpose of this paper is to show that this modification extends the similarity between the adiabatic model and the shell model and indicates some continuity in parameters in going from nucleus to nucleus.

2. TRIAXIAL ADIABATIC CALCULATION

The single-particle wave functions are obtained by diagonalizing the matrix R in a $2s$-$1d$ representation. Here R is the difference between the total Hamiltonian and the spherical harmonic-oscillator Hamiltonian. That is,

$$R = -2\vec{l}\cdot\vec{s} + \tfrac{1}{3}\eta[-q_0^2 + (1.5)^{1/2}\epsilon(q_2^2 + q_{-2}^2)], \quad (1)$$

where η is the Nilsson parameter,[5] and the quadrupole operators are given by

$$q_u^2 = (3.2\pi)^{1/2}\beta r^2 Y_u^2 . \quad (2)$$

The harmonic-oscillator length parameter β is given the same value as in the shell-model calculations of the Oak Ridge group, namely $\beta = 0.988A^{-1/3}$ fm^{-2}. The coefficient for nonsymmetric deformation can be expressed in terms of the oscillator frequencies along the nuclear axes as

$$\epsilon = \frac{\omega_x^2 - \omega_y^2}{\omega_x^2 + \omega_y^2 - 2\omega_z^2} . \quad (3)$$

In a triaxial description there are equivalent parameter pairs (η, ϵ) arising just from relabeling the nuclear axes. For instance, ϵ can be kept positive, since interchanging the x and y axes transforms ϵ into $-\epsilon$ and leaves η unchanged. One can also restrict the magnitude of ϵ to be $\leq \frac{1}{3}$, since exchange of the x and z axes by rotation about the y axis leads to

$$\begin{aligned} \eta &= -\tfrac{1}{2}\eta_0(1+3\epsilon_0), \\ \epsilon &= (1-\epsilon_0)/(1+3\epsilon_0), \end{aligned} \quad (4)$$

where (η_0, ϵ_0) is the original parameter pair.

For even-even nuclei, the intrinsic state χ is formed by putting neutron and proton pairs into the lowest single-particle levels in a manner consistent with the exclusion principle. Intrinsic quadrupole moments Q_0 and Q_2 are then calculated as the expectation values of the sums of the single-particle operators q_0^2 and $q_2^2 + q_{-2}^2$, respectively, including added effective charges of $0.5e$ for both neutrons and protons. The moments of inertia for the triaxial rotor are needed to determine the coefficients a_K in the wave function of the adiabatic model

$$\psi_M^I = \left(\frac{2I+1}{2}\right)^{1/2}\{\sum_K a_K[D_{MK}^I + (-1)^{I-K}D_{M-K}^I]\}\chi . \quad (5)$$

The moments of inertia are extracted from the intrinsic state χ with the help of the Inglis cranking

model,[6] in which the expression is

$$\mathcal{I}_\alpha = 2\hbar^2 \sum_{ik} \frac{|\langle i|J_\alpha|k\rangle|^2}{E_i - E_k}. \quad (6)$$

The states k are occupied in χ, while the states i are not.

This procedure is commonly used with Hartree-Fock calculations[7] for the single-particle states. The main difference between the present calculation and the Hartree-Fock calculations is that the latter produce a large energy gap between the occupied and unoccupied single-particle levels. This affects the resulting moments of inertia even if the single-particle orbitals of the two calculations are alike, since the energy differences appear in the denominator of Eq. (6). In the present calculation the effect on the moments of inertia was tested by arbitrarily increasing the energy gap between occupied and unoccupied levels. The dominant effect is to produce a single multiplicative factor for all three moments of inertia and thus determine the energy scale, leaving the wave functions unchanged. The $E2$ properties and energy ratios are therefore not noticeably affected by the gap variation unless the original gap is quite small, as will be discussed in the examples.

3. ENERGY LEVELS AND $E2$ PROPERTIES

This section presents the excitation energies (see Fig. 1) and $E2$ properties for the first five states of the triaxial model ($I = 0, 2, 2, 3, 4$) for the even-even nuclei with $A = 24$, 26, 30, and 32. Table I compares them with experiment[8-12] and with the much more extensive shell-model calculations.[3,4,13,14] The triaxial model is admittedly very incomplete, since other states are known to exist in the region of 4-MeV excitation energy where the 3^+ and 4^+ levels are found, and these can usually be accounted for by the shell-model treatments. Nevertheless, the results of the adiabatic models are of interest because the similarity with the shell-model treatment occurs for a very limited region of parameter values, around ($\eta = +4$, $\epsilon = 0.20$). The single-particle energies and wave functions for this case are given in Table II. No comprehensive parameter search was made for all four nuclei, but this is the best parameter region for ^{24}Mg and small modifications for the other nuclei lead to the values of Table I.

A word of caution is in order concerning the experimental $B(E2)$ values listed in Table I. The spread of values among different experiments is wider than is given by the listed errors. This is because different techniques of measurement do not agree, and also because some values depend on $E2/M1$ mixing ratios. The latter is particularly true for the transition between the $I = 2$ states, for which case the values of Table I could be changed by a factor of 2 if alternative data were chosen. Since no strong argument can be made for the selection of data, Table I is intended primarily for comparison of calculated $B(E2)$ values.

A. ^{24}Mg and ^{32}S

The nuclei ^{24}Mg and ^{32}S have intrinsic states arising from filling the first two or first four single-particle levels, respectively. From Table II one sees that the gap between occupied and unoccupied single-particle levels is about 2.5 MeV.

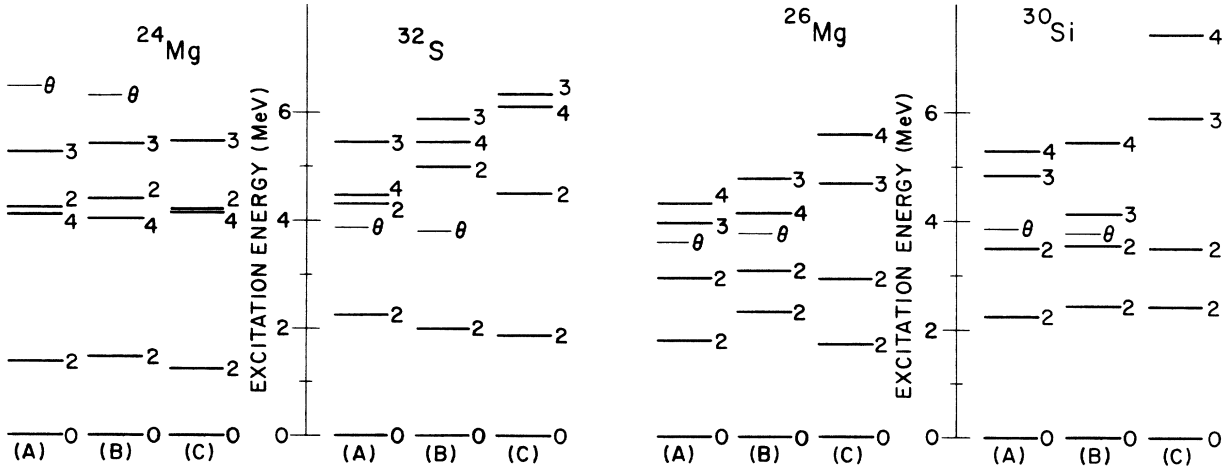

FIG. 1. Energy-level spectra: (A) experimental, (B) shell model, and (C) triaxial model, as explained in the caption of Table I. The line θ refers to the energy above which other levels are found in the experimental and shell-model spectra.

TABLE I. Excitation energies and $E2$ properties: (A) experimental, (B) shell model, and (C) triaxial model with 3 MeV added to the gap and values (η, ϵ) equal to (4, 0.25) for ^{24}Mg, (4, 0.20) for ^{26}Mg, and (3.5, 0.20) for ^{30}Si and ^{32}S. Triaxial energies for ^{26}Mg and ^{30}Si are normalized to the underlined values for $I = 2_2$. Shell-model results are from Refs. 3, 4, 13, and 14. Experimental values are from Refs. 8–12.

	Excitation energy (MeV)				EQ (e fm^2)	$B(E2)$ (e^2 fm^4)				
I	2_1	4_1	2_2	3	2_1	$2_1 \rightarrow 0$	$4_1 \rightarrow 2_1$	$2_2 \rightarrow 0$	$2_2 \rightarrow 2_1$	$3 \rightarrow 2_1$
^{24}Mg										
(A)	1.37	4.12	4.23	5.25	-24 ± 4	85 ± 6	98 ± 50	5 ± 2	10 ± 4	12 ± 6
(B)	1.45	4.04	4.39	5.40	−16	63	82	8	7	12
(C)	1.25	4.17	4.18	5.44	−15	54	77	3	5	5
^{26}Mg										
(A)	1.81	4.33	2.94	3.94	···	74 ± 10	50 ± 7	2 ± 0.5	32 ± 6	···
(B)	2.34	4.12	3.08	4.77	+0.4	68	13	0	97	0
(C)	1.74	5.59	2.94	4.67	−13	56	79	1	20	1
^{30}Si										
(A)	2.24	5.28	3.50	4.83	···	44 ± 7	22 ± 7	7 ± 3	44 ± 25	15 ± 7
(B)	2.42	5.43	3.61	4.12	−6.6	22	5	12	31	0.4
(C)	2.40	7.39	3.50	5.89	+4.6	46	65	2	61	3
^{32}S										
(A)	2.24	4.47	4.29	5.41	-18 ± 5	55 ± 8	81 ± 18	12 ± 4	41 ± 11	13 ± 2
(B)	2.00	5.40	4.97	5.87	−14	43	58	14	15	23
(C)	1.86	6.10	4.50	6.36	−11	35	52	5	14	8

Adding 3 MeV to this gap leaves the wave functions and hence the $E2$ properties essentially unchanged, and leads to the excitation energies listed in Table I. The effect is essentially to halve the moments of inertia, although in comparison with experiment the energy spectrum is somewhat better than one would get by simply halving the original moments of inertia.

It is clear from Table I that the results of the adiabatic model and the shell model are very similar. The components of rotational energy and the coefficients a_K of Eq. (5) are given in Table III. For these nuclei, the wave functions are nearly pure eigenfunctions of K, and the triaxial adiabatic model offers a simple picture for the low-lying states.

B. ^{26}Mg and ^{30}Si

The experimental energy spectra of these nuclei differ from those of the above $T = 0$ cases in that the second 2^+ state lies much lower in energy and becomes the second excited state. In the model they differ from the $T = 0$ cases in that the intrinsic state has a pair of particles or holes in the single-particle levels 3 and 4 of Table II. These two levels are separated by only 0.9 MeV, so variation of the gap has a strong effect on the moments of inertia. If one arbitrarily adds 3 MeV to the gap and fixes the energy scale to fit the second 2^+ level, one obtains the results in Table I. (Alternatively, one could get substantially the same results by adding 5 MeV to the gap which gives a resultant gap about the same as for the $T = 0$ nuclei).

It is clear from Table I that there is much less similarity between the adiabatic model and shell-model calculations for these $T = 1$ nuclei than there is for the $T = 0$ nuclei. The adiabatic model tends to preserve the ratio $B(E2; 4_1 \rightarrow 2_1)/B(E2; 2_1 \rightarrow 0)$ near the value of 10/7 appropriate to $K = 0$

TABLE II. Single-particle wave functions for $(\eta, \epsilon) = (4, 0.20)$. The $2s$ function is positive near the origin. The energy unit is about 1 MeV.

Level	Energy	$\frac{5}{2}\ \frac{5}{2}$	$\frac{5}{2}\ \frac{1}{2}$	$\frac{3}{2}\ \frac{1}{2}$	$\frac{1}{2}\ \frac{1}{2}$	$\frac{5}{2}\ -\frac{3}{2}$	$\frac{3}{2}\ -\frac{3}{2}$
1	−6.09	−0.010	−0.837	0.231	0.487	−0.088	−0.019
2	−3.06	0.032	0.063	0.205	0.187	0.940	0.185
3	−0.35	0.540	0.442	0.406	0.534	−0.219	−0.120
4	0.60	0.761	−0.231	−0.585	−0.080	0.135	−0.010
5	3.16	0.349	−0.181	0.570	−0.575	−0.094	0.429
6	5.74	−0.093	0.116	−0.269	0.325	−0.183	0.876

states despite the fact that the wave functions have strong K mixing, as one sees in Table III. The shell model, on the other hand, gives very weak $B(E2; 4_1 \rightarrow 2_1)$ values and experiment tends to lie somewhere between the calculations. The calculated values for the quadrupole moment of the lowest 2^+ state differ in sign for the two models. Clearly it would be of great interest to measure these quadrupole moments in ^{26}Mg and ^{30}Si.

Despite these differences, there remains a qualitative similarity with observation, particularly with regard to the change in spacing of the 2^+ levels in going from $T=0$ to $T=1$ nuclei. In the adiabatic model the difference results not from a change of deformation, but from the different occupation of the deformed levels. This result differs from the irrotational Davydov model in which the relative moments of inertia, and hence the level spacing, are determined by the asymmetric deformation parameter γ [$\tan\gamma = -\epsilon\sqrt{3}$, where ϵ is defined in Eq. (3)].

4. MAGNETIC DIPOLE EXCITATION

The adiabatic model can also be used to estimate the isovector $M1$ excitation strength of $4N$ nuclei. This property is studied experimentally by scattering electrons inelastically at 180°, and measurements have been made for ^{20}Ne, ^{24}Mg, ^{28}Si, and recently ^{32}S. Generally the strength is concentrated in a few strong peaks at an excitation of about 10 MeV, but the ^{32}S experiment[15] exhibits no large peaks.

In the adiabatic model, the closure sum rule for $4N$ nuclei becomes the simple expression

$$\sum_{\alpha} B(M1; 00 \rightarrow 11\alpha) = 4 \sum_{\mu} \sum_{ik} |\langle i\nu | M^{11}_{\mu 0} | k\nu \rangle|^2 , \quad (7)$$

where the single-particle states k are occupied in the intrinsic state, the states i are unoccupied, and ν refers to neutrons. Since each occupied level contains four nucleons, and the squared matrix elements are the same for neutrons or protons or time-reversed partners, these symmetries are included in Eq. (7). The contribution to Eq. (7) from transitions between particular single-particle levels are given in Table IV for $\eta = 4$, and both axially symmetric ($\epsilon = 0$) and asymmetric ($\epsilon = 0.2$) cases. There are clearly some large matrix elements, particularly the spin-flip transitions ($2 \rightarrow 3$) and ($4 \rightarrow 6$) in the axially symmetric case.

From Table IV one can obtain an idea of the total strength and the energy ordering of the contributions. For example, if ^{20}Ne is represented by a full level 1 in the axially symmetric case, the strength is mostly in the transitions $1 \rightarrow 2$ and $1 \rightarrow 3$. With an axially symmetric adiabatic model, the distribution of strength can be calculated by constructing intrinsic states having $K=1$ and $K=0$ for the $I^\pi = 1^+$, $T=1$ wave functions. However, it is imperative to include the Coriolis-coupling term which mixes states with $\Delta K = 1$. With such calculation one can reproduce the $M1$ transition strengths of shell-model calculations for ^{20}Ne and also for the $1p$ nucleus ^{12}C.

With a triaxial deformation for ^{24}Mg and with levels 2 and 3 filled, Table IV shows the strength to lie mostly in transitions to the lower states $2 \rightarrow 3$ and $2 \rightarrow 4$. For ^{32}S, with a triaxial deformation and filled levels 1–4, there is again considerable strength – now in transitions $4 \rightarrow 5$, $4 \rightarrow 6$, and $3 \rightarrow 5$. The triaxial model shows more frag-

TABLE III. Coefficients $a_K(I)$ of the lowest eigenfunctions and rotational energies $A_i = \hbar^2/2\vartheta_i$ in MeV, for the triaxial cases of Table I. Intrinsic quadrupole values are in $e\,\mathrm{fm}^2$.

	^{24}Mg	^{26}Mg	^{30}Si	^{32}S
$I=2$				
a_0	1.000	0.991	0.769	0.998
a_2	−0.007	−0.131	−0.640	−0.061
$I=4$				
a_0	1.000	0.919	0.690	0.976
a_2	−0.027	−0.395	−0.696	−0.219
a_4	0.000	0.019	0.198	0.005
A_1	0.215	0.338	0.631	0.358
A_2	0.203	0.247	0.319	0.266
A_3	0.942	0.583	0.525	0.967
$\langle Q_0 \rangle$	+25.92	+26.00	+21.25	+20.53
$\langle Q_2 \rangle$	−8.85	−9.29	−17.13	−12.47

TABLE IV. Contributions to the $M1$ isovector sum rule from the indicated transitions between single-particle levels. The values were calculated for $\eta=4$ and either $\epsilon=0$ or $\epsilon=0.20$. The unit is the squared nuclear magneton.

Transition	$\epsilon=0$	$\epsilon=0.20$
$1 \rightarrow 2$	3.19	3.83
$1 \rightarrow 3$	1.56	0.64
$1 \rightarrow 4$	0	0.82
$1 \rightarrow 5$	0.45	0.36
$1 \rightarrow 6$	0.05	0.06
$2 \rightarrow 3$	7.77	4.92
$2 \rightarrow 4$	2.26	4.04
$2 \rightarrow 5$	0.73	0.87
$2 \rightarrow 6$	1.04	0.61
$3 \rightarrow 4$	0	4.55
$3 \rightarrow 5$	4.44	4.74
$3 \rightarrow 6$	0.02	0.80
$4 \rightarrow 5$	0	1.62
$4 \rightarrow 6$	8.79	4.76
$5 \rightarrow 6$	0.00	2.99

mentation of the strength than the axially symmetric model. One would have to include Coriolis coupling to see if the model is capable of predicting the even greater distribution of the strength that seems to be observed experimentally for ^{32}S. It would be of great interest to see what the shell-model calculations give for the distribution of isovector $M1$ strength in ^{24}Mg and ^{32}S.

5. CONCLUSIONS

The reason for comparing the results of the adiabatic model with those of the shell model is to present a pictorial basis for the correlations that the residual interaction produces in the shell-model calculation. For ^{24}Mg and ^{32}S, the triaxial adiabatic model produces results quite similar to those of the shell model. For ^{26}Mg and ^{30}Si the similarity is not so striking, although the triaxial model with virtually unchanged parameters produces a quite different picture for these nuclei, particularly in regard to the $I=2$ states. An experimental determination of the quadrupole moments for these nuclei would be very valuable.

The adiabatic model does indicate that the $M1$ excitation strength in ^{32}S should be comparable to that seen in ^{24}Mg. However, it may be more fragmented, and a calculation of the distribution of such strength via the existing shell-model wave function would be of great interest for comparison with the results of inelastic electron scattering.

The present calculation, which obtains a deformed field via single-particle quadrupole operators and introduces an arbitrary extra gap in the single-particle energies, can be viewed as a pseudo-Hartree-Fock calculation. One should certainly be able to produce results which represent the observations in ^{24}Mg and ^{32}S equally well from a genuine Hartree-Fock calculation. Although there are remnants of similarity, the validity of the triaxial model for ^{26}Mg and ^{30}Si is uncertain in view of the gap dependence of the present results. Furthermore, one should also include the effects of the pairing interaction when two single-particle levels are as close as they are for these nuclei. The triaxial model also fails for ^{28}Si, for which no second low-lying 2^+ state is found experimentally. In this connection it is interesting that the shell-model calculation[4] for ^{28}Si has a second 2^+ state lying 2 MeV below the second experimental 2^+ state.

Finally, while the triaxial model may be pictorially helpful, it is difficult in practice. For odd-A and odd-odd nuclei it would be imperative to include the Coriolis interaction in any adiabatic calculation. The use of the model to select a truncated basis for shell-model calculations is very difficult, although this has been done[16] for ^{24}Mg. Nevertheless, the triaxial adiabatic model does provide a simple method for obtaining some approximate features in nuclei for which the complete shell-model calculation is formidable.

6. ACKNOWLEDGMENTS

The various calculations were greatly simplified by the use of the SPEAKEASY[17] computer language. The author wishes to thank J. B. McGrory and B. H. Wildenthal for some unpublished results of shell-model calculations, and L. W. Fagg for results from electron scattering.

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*Work performed under the auspices of the U. S. Atomic Energy Commission.

[1]E. C. Halbert, J. B. McGrory, B. H. Wildenthal, and S. P. Pandya, in *Advances in Nuclear Physics*, edited by M. Baranger and E. Vogt, (Plenum, New York, 1971), Vol. 4.

[2]B. H. Wildenthal, E. C. Halbert, J. B. McGrory, and T. T. S. Kuo, Phys. Letters 32B, 339 (1970).

[3]B. H. Wildenthal, J. B. McGrory, and P. W. M. Glaudemans, Phys. Rev. Letters 26, 96 (1971).

[4]J. B. McGrory and B. H. Wildenthal, Phys. Letters 34B, 373 (1971).

[5]S. G. Nilsson, Kgl. Danske Videnskab. Selskab, Mat.-Fys. Medd. 29, No. 16 (1955).

[6]D. R. Inglis, Phys. Rev. 96, 1059 (1954).

[7]J. Bar Touv and I. Kelson, Phys. Rev. 138, B1035 (1965).

[8]O. Häusser, B. W. Hooten, D. Pelte, T. K. Alexander, and H. A. Evans, Can. J. Phys. 48, 35 (1970).

[9]S. W. Robinson and R. D. Bent, Phys. Rev. 168, 1266 (1968).

[10]R. D. Symes, B. E. Grossfield, N. Dawson, G. D. Jones, I. G. Main, P. J. Mulhern, M. F. Thomas, and P. J. Twin, Nucl. Phys. A167, 625 (1971).

[11]R. W. Ollerhead, T. K. Alexander, and O. Häusser, Can. J. Phys. 48, 47 (1970); O. Häusser, T. K. Alexander, A. B. McDonald, and W. T. Diamond, to be published.

[12]G. T. Garvey, K. W. Jones, L. E. Carlson, D. A. Hutcheon, A. G. Robertson, and F. F. H. Start, Nucl. Phys. A160, 25 (1971).

[13]B. H. Wildenthal, J. B. McGrory, E. C. Halbert, and H. D. Graber, Phys. Rev. C 4, 1708 (1971).

[14]B. H. Wildenthal, J. B. McGrory, E. C. Halbert, and P. W. M. Glaudemans, Phys. Letters 26B, 692 (1968).

[15]L. W. Fagg, W. L. Bendel, L. Cohen, E. C. Jones, Jr., and H. Überall, Bull. Am. Phys. Soc. 15, 1665 (1970); and private communication.

[16]A. Watt, Nucl. Phys. A172, 260 (1971).

[17]S. Cohen and C. M. Vincent, Argonne National Laboratory Physics Division Informal Report No. PHY-1968E, 1968 (unpublished).