Shell-model test of the rotational-model relation between static quadrupole moments $Q(2^+_1)$, $B(E2)$’s, and orbital $M1$ transitions

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Abstract

In this work, we examine critically the relation between orbital magnetic dipole (scissors mode) strength and quadrupole deformation properties. Assuming a simple $K = 0$ ground state band in an even–even nucleus, the quantities $Q(2^+_1)$ (i.e., the static quadrupole moment) and $B(E2)_{0^+_1 \rightarrow 2^+_1}$, both are described by a single parameter—the intrinsic quadrupole moment $Q_0$. In the shell model, we can operationally define $Q_0$(Static) and $Q_0$(BE2) and see if they are the same. Following a brief excursion to the $sd$ shell, we perform calculations in the $fp$ shell. The nuclei we consider ($^{44,46,48}$Ti and $^{48,50}$Cr) are far from being perfect rotors, but we find that the calculated ratio $Q_0$(Static)/$Q_0$(BE2) is in many cases surprisingly close to one. We also discuss the quadrupole collectivity of orbital magnetic dipole transitions. We find that the large orbital $B(M1)$ strength in $^{44}$Ti relative to $^{46}$Ti and $^{48}$Ti cannot be explained by simple deformation arguments.

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I. INTRODUCTION

In this work we will make a comparison of the shell model and the collective model for several quantities that are sensitive to nuclear deformation. These include $B(E2)$’s, static quadrupole moments, and orbital magnetic dipole transitions. This will be a theory versus theory work. Some experimental results are quoted and serve as anchors for our results, but we will not be inhibited by the lack of experimental data in doing these calculations. We plan in the near future to make a more extensive theory–experiment comparison. But there are holes in the experimental data which must be filled.

The main thrust of our work will be to understand the relationship of orbital magnetic dipole transitions to quadrupole deformations in the nucleus. For example, after the experimental discovery in heavy deformed nuclei of the relation between the orbital magnetic dipole strength and nuclear deformation [1], there have been many works which relate the orbital $M1$ (scissors mode) strength to electric quadrupole transition rates ($B(E2)_{0\rightarrow2}$), often assuming that they are proportional to each other [2, 3, 4, 5, 6].

First, though, we shall do survey calculations of $B(E2)$’s and static quadrupole moments in the $fp$ shell to see how well the shell model relates to the simple rotational model of Bohr and Mottelson [7]. In this rotational model, the formulae for $B(E2)$’s and static quadrupole moments involve a single parameter—the intrinsic quadrupole moment. These formulae are, respectively,

$$B(E2) = \frac{5}{16\pi} Q_0^2(B) \left| \langle I_1 K 20 | I_2 K \rangle \right|^2 \quad (1a)$$

$$Q(I) = \frac{3K^2 - I(I + 1)}{(I + 1)(2I + 3)} Q_0(S), \quad (1b)$$

where $B$ and $S$ stand for $B(E2)$ and “Static”, respectively. Here $Q_0$ is the intrinsic quadrupole moment—what we would see in the rotational frame. On the other hand, $Q(I)$ is what we measure in the laboratory. In the simple rotational model, $Q_0(B)$ is equal to $Q_0(S)$.

For the case $I_1 = 0$, $I_2 = 2$, the Clebsch-Gordan coefficient above is 1. For a simple $K = 0$ band in an even–even nucleus, we obtain

$$B(E2)_{0\rightarrow2} = \frac{5}{16\pi} Q_0^2(B) \quad (2a)$$
\[ Q(2^+) = -\frac{2}{7}Q_0(S). \]

Note that the laboratory quadrupole moment has the opposite sign of the intrinsic quadrupole moment—a well known result. It can be understood physically by imagining rotating a cigar (which has a positive quadrupole moment, i.e., prolate) about an axis perpendicular to the line of the cigar. This will trace out a flat pancake shape which is oblate.

We then find that the ratio

\[ \frac{Q_0(S)}{Q_0(B)} = \frac{7}{2} \frac{5}{16\pi} \frac{Q(2^+)}{\sqrt{B(E2)}} = -1.1038705 \frac{Q(2^+)}{\sqrt{B(E2)}}. \]

(3)

II. QUADRUPOLE PROPERTIES IN THE \( sd \) SHELL

Although we will be performing calculations in the \( fp \) shell, we shall here briefly look over the experimental situation in the \( sd \) shell. In Table II we show experimental values of \( Q(2^+) \), \( B(E2) \), and the ratio \( |Q_0(S)/Q_0(B)| \) as given by Eq. (3). We also show the experimental values of \( E(4^+)/E(2^+) \) as a measure of how close we are to the rotational limit of 10/3, or the vibrational limit of 2/1.

| \( {\text{Element}} \) | \( Q(2^+) \) \( [\text{e fm}^2] \) | \( B(E2) \) \( [\text{e}^2 \text{fm}^4] \) | \( |Q_0(S)/Q_0(B)| \) | \( E(4^+)/E(2^+) \) |
|-----------------|-------------|-------------|-----------------|-----------------|
| \( ^{20}\text{Ne} \) | -23 | 340 | 1.377 | 2.600 |
| \( ^{22}\text{Ne} \) | -19 | 230 | 1.383 | 2.634 |
| \( ^{24}\text{Mg} \) | -16.6 | 432 | 0.802 | 3.012 |
| \( ^{28}\text{Si} \) | +16.5 | 320 | 1.018 | 2.596 |
| \( ^{32}\text{S} \) | -14.9 | 300 | 0.950 | 2.000 |
| \( ^{36}\text{Ar} \) | +11 | 340 | 0.658 | 2.240 |
| \( ^{40}\text{Ar}^* \) | +1 | 330 | 0.061 | 1.980 |
Note that the static quadrupole moments of $^{20}\text{Ne}$, $^{22}\text{Ne}$, $^{24}\text{Mg}$, and $^{32}\text{S}$ are negative, while those of $^{28}\text{Si}$ and $^{36}\text{Ar}$ are positive. If we limit ourselves to axial symmetry, this indicates that the first group has prolate ground state bands and the second group has oblate ones. Skyrme II Hartree-Fock results by Jaqaman and Zamick [10] correctly give the signs of all the static quadrupole moments. The small static quadrupole moment of $^{40}\text{Ar}$ is consistent with magnetic moment results of the $^2\!^+$ state by Stefanova et al. [11].

The ratio $|Q_0(S)/Q_0(B)|$ for $^{20}\text{Ne}$ is larger than the rotational limit, 1.377 versus 1; likewise $^{22}\text{Ne}$. In the case of $^{24}\text{Mg}$, $|Q_0(S)/Q_0(B)|$ is smaller than for $^{20}\text{Ne}$ or $^{22}\text{Ne}$, despite the fact that the spectrum is closer to rotational for $^{24}\text{Mg}$. Also surprisingly for $^{32}\text{S}$, the ratio $E(4)/E(2)$ is 2.000, the vibrational limit, for which one might expect a near zero static quadrupole moment. But the ratio $|Q_0(S)/Q_0(B)|$ is 0.950, close to the simple rotational prediction of unity.

In general, it is difficult to correlate $|Q_0(S)/Q_0(B)|$ with $E(4)/E(2)$ assuming a simple axially symmetric rotor.

We should mention that an analysis of the relationship of $Q_0(S)$ and $Q_0(B)$ has already been performed by Bender, Flocard, and Heenen [12] and Bender et al. [13], albeit not for the $fp$-shell nuclei considered here and using a different method. They perform angular momentum projections on BCS–Hartree-Fock states obtained with the Skyrme interaction SLy6 for the particle–hole channel and a density-dependent contact force in the pairing channel [12]. Their calculations are mainly in the $sd$ shell [12] and neutron-deficient lead region [13]. For one nucleus in common, $^{40}\text{Ca}$, their results for 0$p$–0$h$, 2$p$–2$h$, 4$p$–4$h$, 6$p$–6$h$, 8$p$–8$h$, and 12$p$–12$h$ do not differ so much from previous calculations of Zheng, Berdichevsky, and Zamick [14] as far as the intrinsic properties are concerned, but their calculation has the added feature of providing an energy spectrum and expectation values in the laboratory frame.

In Ref. [10], the authors predict that $^{36}\text{Ar}$ is oblate. This is confirmed by the fact that the static quadrupole moment of the $^2\!^+$ state is positive: $+11 e\text{ fm}^2$ [8]. The experimental $B(E2)$ is 340 e$^2$ fm$^4$ and $|\beta_2| = 0.273$ [9]. Using Eq. (3), we find

$$\frac{Q_0(S)}{Q_0(B)} = 0.6505236 . \tag{4}$$

The energy ratio is

$$\frac{E(4^+_1)}{E(2^+_1)} = \frac{4414.36}{1970.35} = 2.240 . \tag{5}$$
These results are consistent with a nucleus not being too rotational.

The corresponding numbers in the calculation of Bender et al. [12] are

\[ Q(2^+_1)_{\text{lab}} = 13 \text{ e fm}^2, \quad B(E2) \uparrow = 220 \text{ e}^2 \text{ fm}^4, \quad \beta = -0.21. \]  

(6)

The calculated ratios are

\[ \frac{Q_0(S)}{Q_0(B)} = 0.9675, \quad \frac{E(4^+_1)}{E(2^+_1)} = 2.6545. \]  

(7)

These calculations [12] give a more rotational picture than experiment. There is a consistency, however, in that a larger ratio \( E(4)/E(2) \) yields a larger ratio \( Q_0(S)/Q_0(B) \).

III. SHELL MODEL CALCULATIONS OF \( B(E2) \) AND \( Q(2^+_1) \), AND HOW THEY RELATE TO THE SIMPLE ROTATIONAL MODEL

We will put the above relation (3) to the test in a shell model approach for the following nuclei: \(^{44}\text{Ti}, {46}\text{Ti}, {48}\text{Ti}, {48}\text{Cr}, \) and \(^{50}\text{Cr} \). We use the OXBASH program [15] and the FPD6 interaction [16].

The nuclei that we have chosen are far from being perfect rotors. Their description falls somewhere between vibrational and rotational. The ratios \( E(4)/E(2) \), which would all be \( 10/3 \) in the simple rotational case, are as follows: 1.922, 2.010, 2.118, 2.459, 2.342, for \(^{44}\text{Ti}, {46}\text{Ti}, {48}\text{Ti}, {48}\text{Cr}, \) and \(^{50}\text{Cr} \), respectively.

We perform shell model calculations in a complete \( fp \) space using the FPD6 interaction. We assign effective charges of 1.5 for the protons and 0.5 for the neutrons. We calculate \( B(E2)_{0_1 \rightarrow 2_1} \) and \( Q(2^+) \) (the laboratory \( Q \), of course) and put them into Eq. (3) in order to get operational values of \( Q_0(S)/Q_0(B) \). The results are given in Table II.

Except for \(^{48}\text{Ti} \), the FPD6 results for the ratios are all greater than 0.9, reading a maximum of 0.9892 for \(^{48}\text{Cr} \). It is somewhat surprising that these ratios are so close to 1, given that the ratios \( E(4)/E(2) \) are much further away from the rotational limit 10/3.

We can also obtain some of the above ratios from experiment. We refer to the compilation of nuclear moments of Stone [8] and of \( B(E2) \)'s by Raman et al. [9]. Taking these experiments at face value, we see that the ratio \( Q_0(S)/Q_0(B) \) reduces to about 0.75 for \(^{46}\text{Ti} \) and \(^{48}\text{Ti} \), but is bigger than 1 for \(^{50}\text{Cr} \).

It should be noted that in the simplest version of the vibrational mode, \( Q_0(S) \) is zero. We can imagine a nucleus vibrating between a prolate shape and an oblate shape, and causing
TABLE II: The quantity $Q_0(S)/Q_0(B)$ as obtained in the shell model with the FPD6 interaction and experiment.

|                | $Q(2^+_1)$ | $B(E2)$ | $Q_0(S)/Q_0(B)$ |
|----------------|------------|---------|----------------|
| **Theory (FPD6):** |            |         |                |
| $^{44}$Ti       | -20.156    | 607.24  | 0.9029         |
| $^{46}$Ti       | -22.071    | 682.06  | 0.9329         |
| $^{48}$Ti       | -17.714    | 560.78  | 0.8257         |
| $^{48}$Cr       | -33.271    | 1378.4  | 0.9892         |
| $^{50}$Cr       | -30.955    | 1219.0  | 0.9787         |
| **Experiment:** |            |         |                |
| $^{44}$Ti       |            | 650     |                |
| $^{46}$Ti       | -21        | 950     | 0.7521         |
| $^{48}$Ti       | -17.7      | 720     | 0.7282         |
| $^{48}$Cr       |            | 1360    |                |
| $^{50}$Cr       | -36        | 1080    | 1.2092         |

the quadrupole moment to average to zero. On the other hand, the $B(E2)_{0_1 \rightarrow 2_1}$ is quite large in this vibrational limit, causing the ratio $Q_0(S)/Q_0(B)$ to be zero or, in more sophisticated vibrational models, quite small.

### IV. RESULTS WITH AN ALTERNATE INTERACTION T0FPD6

For systems of identical particles, e.g., the tin isotopes, which in the simple shell model involve only valence neutrons, one does not get rotational behaviour. One does go closer to the rotational limit when one has many open-shell neutrons and protons. Whereas two identical nucleons must have isospin 1, a neutron and a proton can have both isospin 0 and 1. This suggests that the $T = 0$ part of the nucleon–nucleon interaction plays an important role in enhancing nuclear rotational collectivity.

In this section, we will use an interaction T0FPD6 that is the same as the FPD6 interaction for $T = 1$ states, but vanishes for $T = 0$ states. We thus expect that the rotational
collectivity will be reduced. This interaction serves as a counterpoint of the full interaction in the previous section. It has been discussed before by Robinson and Zamick [21].

We present the results for T0FPD6 in Table III.

| Nucleus | $Q(\frac{2^+}{1})$ [e fm$^2$] | $B(E2)$ [e$^2$ fm$^4$] | $Q_0(S)/Q_0(B)$ |
|---------|-------------------------------|-------------------------|------------------|
| $^{44}$Ti | $-0.880$ | $375.09$ | $0.0502$ |
| $^{46}$Ti | $-8.195$ | $432.81$ | $0.4348$ |
| $^{48}$Ti | $-8.777$ | $401.97$ | $0.4832$ |
| $^{48}$Cr | $-21.437$ | $813.06$ | $0.8299$ |
| $^{50}$Cr | $-20.985$ | $736.60$ | $0.8535$ |

We see that both $Q(\frac{2^+}{1})$ and $B(E2)$ decrease in magnitude, consistent with the above discussion. However, $Q_0(S)$ decreases more rapidly than $\sqrt{B(E2)}$, so the ratio $Q_0(S)/Q_0(B)$ is less for this case than when the full interaction is present. For $^{44}$Ti this ratio is 0.0502, close to the vibrational limit of zero. For $^{48}$Cr the ratio decreases from 0.9892 to 0.8299; nevertheless, it is still substantial, indicating that the $T = 1$ interaction, acting alone, can lead us to some extent in the direction of the rotational limit.

V. RANDOM INTERACTION STUDIES

Nuclei in the region we are considering have undergone Random Interaction studies. We refer to the works of Velázquez et al. [17] and Zelevinsky and Volya [18]. These works were stimulated by that of Johnson, Bertsch, and Dean [19].

In particular, in the work of Zelevinsky, a quantity is considered which is proportional to the square of $Q_0(S)/Q_0(B)$ and which is normalized to $(2/7)^2$ if $Q_0(S)/Q_0(B)$ equals 1. He calls this the Alaga ratio. He selects cases for which the random interaction yields a $J = 0, J = 2$ sequence of lowest energies. For these he finds two peaks, one corresponding to $Q_0(S)/Q_0(B) = 1$ and the other to $Q_0(S)/Q_0(B) = 0$. In our terminology, these would correspond to the rotational limit in the former case and either the simple vibrational limit
or the spherical limit in the latter case. He cites early work of R. Rockmore [20] as affording an explanation of this surprising behaviour.

VI. ORBITAL MAGNETIC DIPOLE TRANSITIONS IN $^{44}$Ti, $^{46}$Ti, AND $^{48}$Ti

The orbital magnetic isovector dipole transitions, i.e., scissors mode excitations, also display collective behaviour [1]. There are systematics which suggest that $B(M1)_{\text{orbital}}$ is roughly proportional to $B(E2)$. There are more detailed sophisticated relations as well. If one uses a simple quadrupole–quadrupole interaction, the energy weighted $B(M1)_{\text{orbital}}$ is proportional to the difference $(B(E2)_{\text{isoscalar}} - B(E2)_{\text{isovector}})$ [3].

The bare orbital $M1$ operator is

$$\sqrt{\frac{3}{4\pi}} \sum l(i)g_l(i),$$  \hspace{1cm} (8)

where $g_l$ is 1 for a proton and 0 for a neutron. This is the operator that we use in the calculations.

How to extract the scissors mode strength is not completely unambiguous. The mode is associated with low-lying $1^+$ excitations at around 3 MeV. But the strength can be fragmented even at this lowest energy. Besides this, there is orbital strength at higher energies, a somewhat grassy behaviour where individual states are very weakly excited but, because there are so many of them, the total orbital strength can be significant.

Therefore, we will give three sets of values (see Table [IV]). First, we give the strength to the lowest state, then to the lowest 10 states, and finally to the lowest 1000 states (except for $^{48}$Ca, where we include only 300 states). The 10-states strength should encompass what we usually call the scissors mode, while the 1000-states strength is close to the total strength including the grassy, non-collective part. It would appear that the highest excitation energies reached in the experiments [1, 22] are not sufficient to reach the $T+1$ part of the spectrum.

We first discuss the nuclei $^{46}$Ti and $^{48}$Ti, for which there are some data on $B(M1)$. We see consistently that the orbital $B(M1)$ strength is larger in $^{46}$Ti than in $^{48}$Ti. This is consistent with the fact that $^{46}$Ti has a greater $B(E2)$ and static $2^+$ quadrupole moment than $^{48}$Ti.

We next consider the $N = Z$ nucleus $^{44}$Ti, for which there is no data because this nucleus is unstable. The isoscalar orbital $B(M1)$ strength is very weak. This is also true for the spin $B(M1)$, but for a different reason. The isoscalar spin coupling is much smaller than
TABLE IV: The calculated orbital $M1$ strengths ($\mu_N^2$). Unless indicated, the calculations are made with the FPD6 interaction.

|                | $^{44}$Ti | $^{46}$Ti | $^{48}$Ti | $^{48}$Ti/$^{46}$Ti | $^{48}$Cr |
|----------------|-----------|-----------|-----------|---------------------|-----------|
| $T \rightarrow T$ |           |           |           |                     |           |
| Lowest state    | 0.0017    | 0.305     | 0.105     | 0.3443              |           |
| Lowest 10 states| 0.0320    | 0.5979    | 0.3056    | 0.5111              |           |
| Lowest 100 states|          | 0.79      | 0.504     | 0.6380              |           |
| All states      | 0.0355    | 0.9195    | 0.7191    | 0.7820              |           |
| All states (T0FPD6) | 0.0583 | 0.2166    | 0.2235    | 1.0319              |           |

| $T \rightarrow T + 1$ |           |           |           |                     |           |
| Lowest state    | 0.862     | 0.0991    | 0.0041    | 0.4450              | 0.784     |
| Lowest 10 states| 1.4317    | 0.368     | 0.1951    | 0.5302              | 1.3855    |
| Lowest 100 states|          | 2.12      |           |                     | 1.994     |
| All states      | 2.127     | 0.5616    | 0.3099    | 0.5518              | 2.271$^a$ |
| All states (T0FPD6) | 1.1118 | 0.3940    | 0.1671    | 0.4241              |           |

$^a$Lowest 300 states

the isovector one. For the orbital case, the couplings are equal because the operator is $\sum_{\text{protons}} \vec{\ell}$. For the orbital case, the $B(M1)$ isoscalar is very weak because the correlations due to the nuclear interaction move the ground state towards the $SU(4)$ limit, in which $LS$ coupling holds and for which the ground state is a pure $L = 0$ state. For this extreme case, the $B(M1)$ orbital isoscalar will vanish.

The transitions of interest for $^{44}$Ti are, therefore, the isovector orbital dipole ones. The $(T \rightarrow T + 1)$ $B(M1)_{\text{orbital}}$ summed strength is larger in $^{44}$Ti than the $(T \rightarrow T)$ and $[(T \rightarrow T) + (T \rightarrow T + 1)]$ strengths in $^{46}$Ti and $^{48}$Ti, which are 0.5615 (1.4810) and 0.3099 (1.0288) $\mu_N^2$, respectively. On the other hand, $^{44}$Ti is not more deformed than $^{46}$Ti. According to Raman et al. $^9$, the values of the quadrupole deformation parameters $\beta$ for $^{44,46,48}$Ti and $^{48,50}$Cr are, respectively, 0.27, 0.317, 0.269, 0.335, and 0.293. Thus, we have here in $fp$-shell nuclei a counter-example to the experimentally established proportionality between the orbital $B(M1)$ and the $B(E2)$ in heavy deformed nuclei. Perhaps there are correlations
which cause an enhancement for \( N = 2 \) nuclei.

An analysis by Retamosa et al. \[23\] in the \( sd \) shell comparing \( ^{20}\text{Ne} \), \( ^{22}\text{Ne} \), and \( ^{24}\text{Mg} \) was performed (somewhat analogous to \( ^{44}\text{Ti} \) and \( ^{46}\text{Ti} \) for the first two cases), but no anomaly was reported there. In the \( SU(3) \) model, they found consistency in the relation of \( B(M1)_{\text{orbital}} \) to deformation. In this limit, the summed \( M1 \) strengths (all orbital) for \( ^{20}\text{Ne} \), \( ^{22}\text{Ne} \), and \( ^{24}\text{Mg} \) were 1.1, 1.17, and 1.6 \( \mu^2 \), respectively. Looking at the Raman tables \[9\] for these nuclei, there is some complication—the deformation parameters \( \beta_2 \) are not in one-to-one correspondence with the \( B(E2) \)’s. The values of \( (B(E2), \beta) \) for these three nuclei from the Raman tables \[9\] are, respectively, \((0.034, 0.728)\), \((0.0236, 0.562)\), and \((0.0432, 0.606)\), where the units for \( B(E2) \) are \( b^2 \). The authors also do calculations with a more realistic interaction, but no enough strengths are listed in order to make a comparison for the point we are trying to make. Retamosa et al. \[23\] also give strengths to the first 10\(^+ \) states in \( ^{44}\text{Ti} \); our numbers are consistent with theirs.

Earlier works on the shell model for light nuclei include L. Zamick \[24\] and A. Poves \[25\].

VII. CLOSING REMARKS

In this work we have examined what predictions the shell model make for collective properties which are after dealt with in the rotational model. Although the nuclei are far from perfect rotors, the calculated ratio \( Q_0(S)/Q_0(B) \) is fairly close to 1 in many cases. When the FPD6 interaction is used, the orbital magnetic dipole transitions for \( ^{46,48}\text{Ti} \) also fit into this picture, although there is the added complication of separating the collective from the non-collective part in this case. Also there is a substantial enhancement for the \( N = Z \) nucleus \( ^{44}\text{Ti} \), which cannot be explained as purely a deformation effect. We hope our work will stimulate more experimental investigations. There is information of \( B(M1) \) rates in \( ^{46}\text{Ti} \) and \( ^{48}\text{Ti} \), but thus far the orbital \( B(M1) \) has only been extracted in \( ^{48}\text{Ti} \). However, in a short time, we will be able to make a more extensive theory–experiment study of these magnetic dipole transitions.
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