Evidence for Tetrahedral Structure of Calcium-40

N. S. Manton

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Wilberforce Road, Cambridge CB3 0WA, U.K.

Abstract

More than 100 excited states of the Calcium-40 nucleus, with isospin 0, are classified into rotational-vibrational bands of an intrinsic tetrahedral structure. Almost all observed states below 8 MeV can be accommodated, as well as many high-spin states above 8 MeV. The bands have some similarity to those classifying states of Oxygen-16, but the A-mode vibrational frequency is lower relative to the E-mode and F-mode frequencies than in Oxygen-16. Previously identified rotational bands up to spin 16 and energy above 20 MeV are unified here into a smaller number of tetrahedral bands.

1email: N.S.Manton@damtp.cam.ac.uk
1 Introduction

It was proposed nearly 100 years ago that the intrinsic structure of the doubly magic Oxygen-16 nucleus is tetrahedral and that the nucleus is a cluster of four alpha particles [1, 2, 3]. The principal evidence is the presence of low-lying $J^P = 3^-$ and $J^P = 4^+$ states with their excitation energies having the approximate ratio $\frac{5}{3}$, as expected for a tetrahedral rotational band where the collective rotational energy scales as $J(J + 1)$, and the absence of a $2^+$ state below the $3^-$ state. The strong transitions between the $3^-$ state and the $0^+$ ground state, and between the $4^+$ state and the ground state provide further evidence for collectivity. Interpreting the $3^-$ state as a 1-phonon, octahedral vibration of an intrinsically spherical nucleus is less convincing, because there is no obvious multiplet of close-to-degenerate 2-phonon states with spin/parities $6^+, 4^+, 2^+, 0^+$.

Lezuo in the 1970s drew attention to similar features in the energy spectrum of the two larger magic nuclei Calcium-40 and Lead-208 [4]. Calcium-40 has a low-lying $3^-$ state, and then three $4^+$ states in the required energy range for a ratio $\frac{5}{3}$, but one has energy 15% too low and the other two have energy 5% too high. Lezuo mentioned that a fuller understanding of the spectrum would require a modelling of vibrational modes. This is what we initiate here. In Lead-208, the yrast $4^+$ state has the right energy to be associated with the well known yrast $3^-$ state, and Heusler has argued that eight additional states appear to lie in collective tetrahedral bands [5].

The analysis of vibrations coupled to rotations has been quite energetically pursued in the case of Oxygen-16. It was initiated by Wheeler [1] and by Dennison [6], and followed up by Robson [7], Bijker and Iachello [8], and others. The most detailed model was constructed recently by Halcrow, King and the present author [9, 10]. Our model was based on Skyrme solutions [11] in which alpha particles are extended structures of the Skyrme field, stabilised by their topological charge (baryon number). Four of these extended alpha particles retain their identities and only slightly merge, forming a stable tetrahedral structure that is the basis for Oxygen-16 [12]. This is not very different from the more familiar tetrahedral cluster of pointlike or spherical alpha particles.

A tetrahedron of alpha particles can vibrate and rotate. The vibrational modes of four particles connected by springs give a reasonable approximation to the vibrational modes of a tetrahedral Skyrmion with baryon number 16. There are A-, E- and F-mode vibrations: the A-mode is non-degenerate and preserves the tetrahedral symmetry, the E-mode is a doubly-degenerate quadrupole mode, and the F-mode is a triply-degenerate vector mode. Their frequencies (energies, as we set $\hbar = 1$) are, respectively, approximately 12, 3.5 and 6 MeV. The simplest quantised model of the dynamics has multiple phonon states of these modes, coupled to rotations. These are known as rovibrational (rotational-vibrational) states. Each vibrational state generates a rotational band, whose allowed spin/parities are well known in molecular physics [13].

In Oxygen-16, the E-mode has lowest frequency, and in [9, 10] the first excited $0^+$
state at 6.05 MeV is interpreted as a state with two E-phonons. The E-mode, if extended to large amplitude, can deform a tetrahedron of four alpha particles through a square configuration into the dual tetrahedron (the spatial inversion of the initial tetrahedron). As the intermediate square configuration has higher energy, this is quantum mechanically a tunnelling process. Its importance has been long recognised [6]. Without tunnelling, the Oxygen-16 spectrum would have many parity doublets, but the tunnelling splits these, matching the data. In [9] we constructed a two-dimensional E-manifold, which extended the space of E-mode vibrations so as to include tetrahedral configurations of both types and square configurations. Quantum mechanics on this E-manifold replaces the harmonic oscillator quantisation of the E-mode, but states can still be classified in terms of E-phonons (by examining the wavefunctions close to the initial tetrahedral configuration). The contributions of A-phonons and F-phonons were added in [10]; these were treated harmonically.

By combining E-manifold states with A- and F-phonons, and rotations, we obtained a spectrum of isospin 0 states of Oxygen-16, classified by their spin/parity and energy, matching just about every known state of Oxygen-16. The matching is precise up to 15 MeV above the ground state – there is just one predicted 4− state with energy 13 – 14 MeV that has not been observed. Above 15 MeV, more states are predicted than have been observed, but the experiments are rather incomplete here, and the analysis difficult. For example, our theory predicts a few 6− states between 15 and 20 MeV, but none has yet been observed, partly because such states are inaccessible to some of the experiments. Several 6+ states are known in this range, and it is likely that 6− states are present too. Between 20 and 30 MeV several high-spin states have been seen, up to spin 9 and maybe spin 10. These are also predicted by our model, but the match to energies, and even to the number of states, is not very good.

One surprise in all this is that there appears no need to identify any states as shell-model excitations. They are all collective. Alternative descriptions of the excited states of Oxygen-16 are available, entirely in terms of the shell model, see e.g. [14], p.7. The conclusion seems to be that collective excitations and shell-model excitations are alternative ways of modelling the same nuclear states, and it is not necessary to treat them as independent. The reason seems to be the strong mixing that occurs between pure shell-model excitations. This applies even for the lowest-energy 1-particle, 1-hole (1p1h) excitations. By contrast, in the isospin 1 sector of Nitrogen-16, Oxygen-16 and Fluorine-16, the lowest states are clearly a quartet of simple 1p1h excitations, with very similar energies. The particles are in the d_{5/2} and s_{1/2} states of the sd-shell, and the holes are in the p_{1/2} states of the p-shell. Combined, they give states with spin/parities 3−, 2−, 1−, 0− [15]. States with the same spin/parities should also occur with isospin 0 in Oxygen-16, and they do, as yrast states, but with a greater spread of energies. However, these states are also easily identifiable with collective states, contributing to rotational bands. For example, the lowest 1− state is the bandhead of the F-band, with one F-phonon. If this state were identified purely as a shell-model state, it would spoil the interpretation of several higher-spin, higher-energy states as lying in this F-band. The only state whose 1p1h character appears to have a dominant influence is the yrast
0\textsuperscript{−} state. In the collective interpretation, this state has three E-phonons, and a rather complicated E-manifold wavefunction with rather high energy. The overlap with a 1p1h wavefunction should reduce its energy closer to the observed value.

Let us turn now to Calcium-40. Finding a Skyrmion with baryon number 40 to model Calcium-40 has been difficult, but using a suitable multi-layer structure as starting point for a numerical relaxation, a tetrahedrally symmetric solution was found [16]. This solution is shown in Figure 1 in two orientations. It resembles the tetrahedral Skyrmion of baryon number 56 [17] (56 is a tetrahedral number), with four clusters of baryon number 4 chopped off at the vertices. The final structure is closer to spherical, without the pointedness of an ideal tetrahedron, and therefore more stable.

This Skyrmion solution also emerges by stacking 40 basic Skyrmions of baryon number 1 in a cluster with tetrahedral symmetry. A structure like this arises as a subcluster of the FCC lattice, or as a weight diagram of a representation of SU(4) (all SU(4) weight diagrams have at least tetrahedral symmetry) [18, 19]. A model of the relevant cluster is shown in Figure 2, in the same orientations as for the Skyrmion. The steel balls correspond to the cores of the basic Skyrmions, and the magnetic rods connecting them correspond to the nearest-neighbour attractive forces – these are not materially present in the Skyrmion solution. Physically, such a cluster appears as a static solution in a variant of the Skyrme model called the lightly bound model, where the basic Skyrmions attract but hardly merge [20, 21]. It is particularly clear in the lightly bound model how to orient the basic Skyrmions to achieve maximal attraction and greatest stability. The Skyrmion in Figure 1, which is a solution of the standard Skyrme model (with sigma model term, Skyrme term, and pion mass term in the Lagrangian), can be obtained by relaxation of its analogue in the lightly bound model.

Notice that the Skyrmion in Figure 1 has the property that it can be identified as...
a bound cluster of 10 distinct tetrahedral Skyrmins of baryon number 4, i.e. Skyrme model alpha particles. These tetrahedral subclusters are highlighted by yellow magnetic rods in Figure 2.

We will not use the Skyrmion in our later discussion, but it is encouraging that a tetrahedrally symmetric, quasi-spherical Skyrmion with baryon number 40 exists. Instead, we will present a phenomenological model of states of Calcium-40, based on the rovibrational spectrum of a tetrahedron. This will involve A-, E- and F-phonons, combined with rotations. The model here is less detailed than the model for Oxygen-16 in [10], but qualitatively similar.

One significant difference, compared with Oxygen-16, is that states of Calcium-40 have been classified up to spin 16, whereas for Oxygen-16 the highest confirmed spin is about 9. Such high spins have not been measured directly, but inferred from gamma-ray spectra. We make substantial use of the interesting and detailed spectra of Calcium-40 states with positive parity, up to 16+, that have been tabulated and gathered into proposed rotational bands in [22]. There, no use is made of the theory of tetrahedral vibrations. The negative parity states are less completely classified, but we use the spectra tabulated and gathered into bands in [23]. There again, a tetrahedral structure is not discussed, but it is argued that some type of permanent octupole deformation needs to be considered. For the complete set of experimentally determined states we use the standard compilation [24].

Perhaps our most important observation, providing evidence for the tetrahedral structure of Calcium-40, is that the number of states in two of the rotational bands with even spin and positive parity, described in [22], jumps by one starting at 8+ and jumps by one again starting at 14+. This is just as expected for the single rotational band of a tetrahedron excited by one E-phonon, in contrast with rotational bands of an ellipsoidally deformed nucleus, where there are no such jumps. More generally, we show that several of the rotational bands identified in [22] and [23] are naturally unified into far fewer bands when interpreted as rovibrational excitations of a tetrahedron.

Four states of Calcium-40 can be clearly identified as 1p1h excitations. The particle states are from the f7/2 shell and the holes are d3/2 states from the sd-shell. Combined,
they give states with spin/parities $5^-, 4^-, 3^-, 2^-$. Their energies, and even their ordering, are not easily or precisely predicted by shell-model calculations \[15\], but the trend is for the energy to decrease as the spin increases. In particular, the $5^-$ state, identified with the observed yrast $5^-$ state at 4.491 MeV, is strikingly low in energy.

These four $1p1h$ states of Calcium-40 are not easily fitted into collective rotational bands. However, our model for Oxygen-16 suggests that they do not need to be treated as additional to the collective states. We will show later that it is best to identify these four states as belonging to rotational bands, but with significantly displaced energies. As collective states, they have wavefunctions and energies that are significantly affected by their overlap (superposition) with pure $1p1h$ excitations, but we do not need to postulate that they are totally distinct. The effect is largest for the $5^-$ state. In our model it lies in the E-band, with one E-phonon, but its energy is shifted down by more than 2 MeV compared to what would be expected by extrapolation from other states in the E-band.

2 Rovibrational bands of a tetrahedron

Here we review the allowed spin/parities of rovibrational states of a vibrationally excited tetrahedron. They are obtained by using the character table of the tetrahedral group $T_d$ \[25\], which is reproduced as Table 1 in Appendix A. Spins up to 12 are tabulated in \[13\], p.450 but we need some results up to spin 16.

The group $T_d$ has five irreducible representations (irreps), denoted $A_1$, $A_2$, $E$, $F_2$, $F_1$, where $A_1$ (the trivial irrep) and $A_2$ are 1-dimensional, $E$ is 2-dimensional, and $F_2$ and $F_1$ are 3-dimensional. It appears that, as for Oxygen-16, the dominant vibrational modes of the intrinsic tetrahedron modelling Calcium-40 are $A$-, $E$- and $F$-modes, transforming according to the $A_1$, $E$ and $F_2$ irreps. 1-phonon states are classified by these three irreps.

Multiphonon states also occur. As phonons are bosons, multiphonon states transform as a symmetrised tensor product of 1-phonon irreps. These reducible representations of $T_d$ can then be decomposed into irreps. Particularly important for us is that the space of vibrational states with two E-phonons decomposes as

$$E^2 = A_1 \oplus E.$$  \hspace{1cm} (2.1)

(For a representation $d$ with character $\chi$, the symmetric square $d^2$ – we drop the subscript “symm.” – has character $[\chi^2](g) = \frac{1}{2} \{ \chi(g)^2 + \chi(g^2) \}$ for each group element $g$.) See \[10\] or \[13\] p.127 for higher symmetrised powers of $E$.

To find the allowed spin/parities of the rotational excitations of a given vibrational state, one starts with the characters $\chi$ of the spin $J$ representation of the group O(3) with positive or negative parity ($J$ is always an integer here). For a pure rotation by angle $\theta$, the character is

$$\chi(\theta) = \frac{\sin(J + \frac{1}{2})\theta}{\sin \frac{1}{2}\theta}.$$  \hspace{1cm} (2.2)
for either parity. For a rotation by \( \theta \) combined with an inversion \( I \) it is

\[
\chi(\theta, I) = \pm \frac{\sin(J + \frac{1}{2})\theta}{\sin \frac{1}{2}\theta}
\]

with the upper (lower) sign for positive (negative) parity. Next, these spin \( J \) characters need to be restricted to the elements of the group \( T_d \), which lie in five conjugacy classes – rotations by 0, \( \frac{2\pi}{3} \) and \( \pi \), and rotations by \( \pi \) and \( \frac{\pi}{2} \) combined with inversion. The characters of the spin \( J \) representation of \( O(3) \) thereby become characters of a (generally reducible) representation of \( T_d \), and using the character table one can find its decomposition into irreps. If an irrep \( d \) occurs here and simultaneously as an irrep of a multiphonon excitation (as for example, on the right hand side of (2.1)), then that multiphonon excitation can have a rovibrational state of spin \( J \) and the appropriate parity. If \( d \) occurs with multiplicity \( n \) then the spin \( J \) state occurs with multiplicity \( n \).

For example, the spin 2, positive parity representation of \( O(3) \) is 5-dimensional and its characters for the five tetrahedral conjugacy classes are, respectively, 5, \( -1 \), \( 1 \), \( 1 \), \( -1 \).

\[
\text{(2.4)}
\]

so \( 2^+ \) states occur in the rovibrational E-band (one E-phonon) and in the F-band (one F-phonon), and also in multiphonon rovibrational bands where the multiphonon state has an irrep E or F in its \( T_d \) decomposition.

Using the formulae (2.2) and (2.3), and the \( T_d \) character table, one finds that the ground state band, the rotational excitations of a tetrahedron with no vibrational phonons, has states with spin/parities

\[
\text{g.s.band : } 0^+, 3^-, 4^+, 6^+, 6^-, 7^-, 8^+, 9^+, 9^-, 10^+, 10^-, 11^-, 12^+, 12^-, 13^+, 13^-, 14^+, 14^-, 15^+, 15^-, 16^+, 16^-, 17^+, 17^-, 18^+, 18^-, \ldots
\]

(2.5)

(Note that multiplicities greater than 1 start at spin 12.) There is some periodic structure here. Whenever the spin increases by 6, the number of allowed states (ignoring the parity label) increases by 1. So, for example, there are no spin 2 states, one spin 8 state and two spin 14 states. This is because the characters of \( O(3) \), for rotations by \( \frac{2\pi}{3} \) and \( \pi \), repeat when \( J \) increases by 6, whereas the character for the trivial rotation by 0, which is \( 2J + 1 \), increases linearly with \( J \). Similarly, the difference between the number of positive parity and negative parity states has period 4 as \( J \) increases, being 1, 0, 0, –1 for \( J = 0, 1, 2, 3 \mod 4 \). This is because the characters for the rotations by \( \pi \) and \( \frac{\pi}{2} \), combined with inversion, repeat when \( J \) increases by 4.

There is another feature of the states in the ground state band (2.5). The set of allowed spins (ignoring the parity labels and the multiplicities) forms a numerical semigroup [26]. This is explained in Appendix B.

The next important band is the E-band, the rovibrational states where the tetrahedron is excited by one E-phonon. Here the states all occur symmetrically as parity
doubles. The allowed spin/parities are

\[ \text{E-band : } 2^\pm, 4^\pm, 5^\pm, 6^\pm, 7^\pm, 8^\pm, 9^\pm, 10^\pm, 11^\pm, 12^\pm, 12^\pm, 13^\pm, 13^\pm, 14^\pm, 14^\pm, 14^\pm, 15^\pm, 15^\pm, 16^\pm, 16^\pm, \ldots \]  \hspace{1cm} (2.6)

In the E-band, the number of states of each parity increases by 1 whenever the spin \( J \) increases by 6. In particular, there is an upward step in the number of allowed states at spin 8 and spin 14, and these steps are observed experimentally \[22\]. For low spins, the energies are higher in the E-band than in the ground state band because of the E-phonon energy, but the bands cross over at higher spin, because the phonon stretches the nucleus, increasing its effective moment of inertia.

A further band is the 2-phonon, \( E^2 \)-band. As pointed out in eq.\((2.1)\), \( E^2 = A_1 \oplus E \). The \( A_1 \) irrep is trivial, so 2-phonon states transforming under this irrep have rotational excitations with the same spin/parities as in the ground state band, \( (2.5) \). 2-phonon states transforming under the \( E \) irrep have rotational excitations with spin/parities as in the E-band, \( (2.6) \). The energies are slightly higher for the 2-phonon than 1-phonon states, and the E-band and \( E^2 \)-band appear not to cross over.

The triply-degenerate vibrational states with one F-phonon have a vectorial character, and carry an internal spin/parity \( 1^- \). Their rotational excitations combine a spin/parity \( J^P \) from the ground state band \( (2.5) \) with the internal spin/parity \( 1^- \), using the usual Clebsch–Gordon rules. This gives the F-band spin/parities

\[ \text{F-band : } 1^-; 2^+; 3^+; 4^+; 3^-; 4^-; 5^-; 5^\pm; 6^\pm; 7^\pm; \ldots \]  \hspace{1cm} (2.7)

where the states are grouped according to their ground state band spin/parity, i.e. the values \( 0^+, 3^-, 4^+, 6^\pm, \ldots \). Because of the relatively high energy of the F-phonon, we do not need to consider higher spins here.

### 3 Interpreting the Calcium-40 spectrum

As primary data for the spectrum of excited states for Calcium-40 we use the ENSDF adopted levels \[24\]. We have assigned 104 of these states to tetrahedral rovibrational bands. The assignments are listed in Table 2 of Appendix C, and the energies and spins of the states are shown in Figure 3. Filled circles (triangles) indicate positive (negative) parity states, and the colouring distinguishes the various rovibrational bands. States with a given spin, in one band, do not all have the same energy. We saw this in Oxygen-16, where the energy splittings could be calculated \[9,10\]. Part of the splitting between positive and negative parity states arose from the tunnelling between a tetrahedral configuration and its dual. We have not made new calculations for the splittings here, as we do not have a precise dynamical model for the tetrahedral deformations.

From \[24\] we retain almost all states below 8 MeV. The states at 6.160, 6.422, 7.421 and 7.481 MeV are dropped as they are either doubtful or have unknown (low) spins. The states at 7.658 and 7.694 MeV are dropped as they have isospin 1. Above 8 MeV we retain selected states, mainly of spin 5 and higher. States of lower spin are
Figure 3: Observed Calcium-40 energy spectrum, with the rovibrational band assignments in our model. Positive parity states are displayed as filled circles, negative parity states as filled triangles. (E2- denotes the negative parity part of the E$^2$-band, etc.)
numerous and would lie in multiphonon bands, and we have only attempted to classify a few of these. In several cases, in the range between approximately 7 and 10 MeV, the experiments only partially constrain the possible spin and parity of a state. In these cases, we have made a choice that seems most consistent with the pattern of bands that we have partially determined using other states. These choices are shown in Table 2 and in Figure 3. Most of them are for states classified as having two phonons.

Above 9 MeV, high-spin states have their energy and spin mainly inferred from the pattern of gamma decays, rather than direct measurement, and we retain all the states that have been assigned to bands in [22] and [23]. The highest of these is a 16$^+$ state at 22.106 MeV.

The band assignment that we are most confident about is the E-band. We can identify 31 observed states up to spin 16, of positive and negative parity, as being in this band. They are shown in blue in Figure 3. Many are from the positive parity bands 2, 3 and 4 as identified in [22], and from the negative parity bands in [23] (rightmost two columns in Fig. 5). Just a few expected states of positive parity are missing from this E-band – a second 11$^+$ state, a second 15$^+$ state, and a second and third 16$^+$ state are expected, according to the list (2.6), but have not yet been identified. A greater number of negative parity states are missing. This is because there is just one identified state with each of the spin/parities 8$^-$, 10$^-$, 11$^-$, 13$^-$, 15$^-$ in [23], but the E-band requires two. Of more concern is that two 12$^-$ states, and three 14$^-$ and 16$^-$ states are expected, but none of these have been observed or inferred. Maybe a reanalysis of the data, taking these expectations into account, would reveal the missing states.

The plot of energy $E$ against spin $J$ is approximately linear for the E-band. It is nothing like a linear relation between $E$ and $J(J+1)$. Presumably the E-phonon softens the nucleus, and centrifugal stretching produces an effective moment of inertia that increases with $J$. The approximate linearity with $J$ allows us to extrapolate the E-band down in energy towards spin 0. In this way we have identified the 2$^\pm$ and 4$^\pm$ states to be assigned to the E-band. We can also read off the E-phonon frequency to be approximately 2.5 MeV.

The negative and positive parity states are fairly well interleaved in the E-band. An outlier, below the general trend, is the yrast 5$^-$ state at 4.491 MeV. This is interpreted as in the E-band but with lowered energy because of its partial 1p1h character. The 4$^-$ and 2$^-$ states in the E-band are also yrast states, and are interpreted as having a partial 1p1h character, but a less pronounced lowering of energy. The final 1p1h excitation, with spin/parity 3$^-$ cannot be in the E-band at all. It probably contributes to the yrast 3$^-$ state at 3.737 MeV, which is assigned here to the ground state band.

Unifying several of the rotational bands from refs. [22, 23] into one tetrahedral rovibrational band is theoretically attractive, not only because it explains some of the observed jumps of multiplicity as the spin increases. It also appears to be supported by the many cross-band gamma transitions that are observed. For example, transitions of roughly equal strength connect the multiple states with spin above 10 (see Fig. 1 of [22]).
Only a few states can be identified as being in the ground state band. It appears that here the intrinsic shape is more rigid, and that the energy $E$ scales more closely with $J(J+1)$. The $0^+$ ground state and $3^-$ yrast state at 3.737 MeV are clearly in this band, but we suggest that above the $3^-$ state the ground state band crosses the E-band, so that the $6^\pm$, $7^-$ and $9^-$ states in the ground state band are well above those in the E-band. (Our assignment of the $6^-$ state at 9.860 MeV to the ground state band is tentative.) This band crossing is similar to what occurs in Oxygen-16, where the ground state band crosses the E-band between spin 4 and spin 6 \cite{7,10}.

The $4^+$ state at energy 5.279 MeV is a mystery. It occurs at the crossover of the ground state band and the E-band. Uniquely, we have assigned it to both these bands. Really, two independent states are needed for these bands. Possibly the observed state at 6.160 MeV, which has an uncertain $3^-$ spin/parity assignment, and which we have currently omitted from our bands, is the further $4^+$ state we need. Alternatively, we have misassigned the low-lying $4^+$ states. In any case, between 5 and 7 MeV there are apparently just three $4^+$ states observed, but our band structure needs four.

The E-band does not accommodate all the known positive parity states with high spin. In particular, higher-lying observed states with spin/parities $8^+, 10^+, 12^+, 14^+, 16^+$ are in a separate band, shown as band 1 in \cite{22}. We assign them to the E$^2$-band. As noted before in eq. 2.1, the E$^2$-band splits into an $A_1$ part and an E part. In modelling Oxygen-16 we discovered that the $A_1$ part has clearly lower energy, and we assume the same holds for Calcium-40. So the high-spin states listed above are in a band with the same spin/parities as in the ground state band. We assume this is again a rather soft band, with an approximately linear relationship between $E$ and $J$. The energies in this $A_1$ part of the E$^2$-band are lower than those of the ground state band for spins down from 16 to 6, but then the bands cross. By extrapolating down to spin 0, we identify the second excited $0^+$ state at 5.212 MeV as the E$^2$-bandhead. Its energy matches our estimate for the energy of two E-phonons rather well.

The high-spin states in the E part of the E$^2$-band have not been identified – they would include, for example, further $14^+$ states. But a few low-spin states in this part of the band can be identified, in particular the states with spin/parity $2^\pm$.

We need an interpretation for the first excited $0^+$ state at energy 3.353 MeV. This is assigned as the A-bandhead, a state with one A-phonon. The A-phonon energy is therefore approximately 3.4 MeV, somewhat higher than the E-phonon energy. The A-band is assumed to be less soft than the bands with one or two E-phonons, because the nuclear shape stays closer to spherical. Like the $A_1$ part of the E$^2$-band, the A-band has the spin/parities of the ground state band, and we can identify its $3^-$ and $4^+$ states, and possibly its $6^+$ state, all having energies about 3 MeV higher than those in the ground state band. However, there is a shortage of observed $6^+$ states in the required energy range, and a worse shortage of $6^-$ states.

A further band that we recognise is the F-band, with spin/parities as in (2.7). This includes the $1^-$ and $3^+$ yrast states at 5.903 and 6.030 MeV, which cannot occur in other bands. Using the energies of these two states we estimate the F-phonon energy to be about 5 MeV, higher than the E-phonon and A-phonon energies. We have identified
states in the F-band up to spin 5 and just beyond, but with considerable uncertainty.

Above the F-band we find evidence for an $A \times E$ band, an $A \times F$ band, and an $E \times F$ band. The allowed spin/parities in the $A \times E$ band are the same as in the $E$-band, starting with $2^\pm$ and $4^\pm$, and those in the $A \times F$ band are as in the $F$-band, starting with $1^-$ and $2^+$. Those in the $E \times F$ band are parity doubles of the states in the $F$-band, as $E \times F = F_1 \oplus F_2$, so the first few are $1^\pm$, $2^\pm$, and then $3^\pm$ with multiplicity two. The energies of all these states are estimated to be the sum of the energies of the two contributing phonons and the spin energy. (Recall that the $A$-, $E$- and $F$-phonons have approximate energies 3.4, 2.5 and 5 MeV, respectively.) Suitable states to place in these bands can be tentatively assigned, by making appropriate choices among the spin/parity assignments in [24]. These choices are shown in Table 2 and Figure 3. Rather a lot of choices are needed, so some are likely to be incorrect. A few further states with low spins are tentatively assigned to other multiphonon bands, including bands with two $A$-phonons, three $E$-phonons, or two $E$-phonons combined with one $A$-phonon (this last band is omitted from Figure 3). The band with three $E$-phonons is the lowest that can accommodate a $0^-$ state.

4 Conclusions

We have shown that more than 100 observed states of Calcium-40, with isospin 0, can be assigned to rovibrational bands of an intrinsically tetrahedral nuclear structure. This makes Calcium-40 similar to the smaller doubly magic nucleus Oxygen-16. Vibrational $A$-, $E$- and $F$-modes having approximate frequencies 3.4, 2.5 and 5 MeV can be excited, and we have identified states with up to three vibrational phonons. In particular, 31 states are assigned to the band with one $E$-phonon. Relative to the $E$-mode and $F$-mode frequencies, the $A$-mode frequency appears to be considerably lower than it is in Oxygen-16. Possibly this is because in Oxygen-16 the $A$-mode is a true breathing mode of the four alpha particles, whereas in Calcium-40 it is more likely to be a tetrahedrally symmetric, volume-preserving vibration, where six alpha particles move outward and four move inward.

Our scheme accommodates almost all observed states with excitation energy below 8 MeV, as well as all the known states of higher energy with spins from 8 up to 16. It explains why there are few observed $0^-$, $1^+$ and $3^+$ states – these can only occur in multiphonon bands (with the exception of one $3^+$ state in the $F$-band). It also explains why $2^+$ states are more numerous than $2^-$ states – the $F$-band and $A \times F$ bands exclude the latter. Similarly, $4^+$ states are more numerous than $4^-$ states because the ground state band and $A$-band exclude $4^-$ states.

The scheme has a few gaps – one more $4^+$ state is predicted between 5 and 7 MeV, and a few extra states of spin 5 and spin 6 are expected between 8 and 11 MeV – these have not yet been observed. A number of extra states with spin 8 or more, particularly of negative parity, are also expected from 11 MeV upwards. One of these is the $8^+$ state in the ground state band, with a predicted energy between 12 and 13 MeV.

The scheme could be made more robust if the spins and parities of 20 states between
about 7 and 10 MeV were better known. At present, it is necessary to make choices among the experimentally allowed values in order to fill some of the higher bands, but these choices cannot be regarded as firm predictions, as there are too many of them.

On the theoretical side, it would be helpful to have more information about the Skyrmion with baryon number 40, especially its low-lying vibrational modes. More generally, it would be helpful to investigate the dynamics of clustering and vibrations in models with 10 alpha particles.

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Appendix A: Character table of $T_d$

The 24 elements of $T_d$ lie in five conjugacy classes, denoted $Id$, $C_3$, $C_2$, $\sigma_d$ and $S_4$. These consist, respectively, of rotations by 0, $\frac{2\pi}{3}$ and $\pi$, and rotations by $\pi$ and $\frac{\pi}{2}$ combined with an inversion. The character table for the five irreps is [25]

|     | $Id$ | $C_3$ | $C_2$ | $\sigma_d$ | $S_4$ |
|-----|------|-------|-------|------------|-------|
| $A_1$ | 1    | 1     | 1     | 1          | 1     |
| $A_2$ | 1    | 1     | 1     | -1         | -1    |
| $E$   | 2    | -1    | 2     | 0          | 0     |
| $F_2$ | 3    | 0     | -1    | 1          | -1    |
| $F_1$ | 3    | 0     | -1    | -1         | 1     |

Table 1: Character table of $T_d$.

Appendix B: Numerical semigroups

It is noteworthy that in the ground state rotational band, the spins that occur form a numerical semigroup [26]. This is the case not just for an object whose intrinsic structure is tetrahedral, with symmetry $T_d$, but for any other symmetry. The allowed spins for, respectively, objects with tetrahedral, cubic and icosahedral symmetries, i.e. $T_d$-symmetry, $O_h$-symmetry and $Y_h$-symmetry, are [27]

\[
T_d : \quad 0, 3, 4, 6, \ldots , \quad \text{(B.1)} \\
O_h : \quad 0, 4, 6, 8, 9, 10, 12, \ldots , \quad \text{(B.2)} \\
Y_h : \quad 0, 6, 10, 12, 15, 16, 18, 20, 21, 22, 24, 25, 26, 27, 28, 30, \ldots . \quad \text{(B.3)}
\]
In each case, the dots ... indicate that all integers beyond the last one shown are present.

A numerical semigroup $S$ is defined as a subset of the non-negative integers that includes 0 and is closed under addition; further, the set $G(S)$ of missing integers – the gaps – is finite. Any $S$ has a (minimal) generating set, with no common factors, such that every element of $S$ is a linear combination of generators with non-negative integer coefficients. For the above examples, the generators are $< 3, 4 >$, $< 4, 6, 9 >$ and $< 6, 10, 15 >$.

The number of gaps $g(S)$ is called the genus, and the highest gap $F(S)$ is called the Frobenius number; they are respectively 3, 6, 15 and 5, 11, 29 in the above examples. $S$ is called a symmetric numerical semigroup if $F(S)$ is odd, and for such $S$ it is a theorem that $F(S) + 1 = 2g(S)$. The examples above are all symmetric. A symmetric numerical semigroup $S$ has the nice property that for each pair of integers $n$ and $F(S) - n$, with $0 \leq n \leq F(S)$, just one of the pair is in $S$ and the other is a gap. This makes it easy to reconstruct the allowed spins from the first few. For example, for $O_h$, if one remembers that the list starts with 0, 4 and 6 and that there are no gaps from 12 onwards, then the only further gaps are at $11 - 0 = 11$ and $11 - 4 = 7$. Similarly, there are only four gaps beyond the element 15 in the $Y_h$ list, at 17, 19, 23 and 29.

Appendix C: Table of Calcium-40 states

Table 2 lists the experimentally observed isospin 0 states of Calcium-40, and their assignment to tetrahedral rovibrational bands in our model. Nearly all the states below 8 MeV are listed and assigned to bands, although a few dubious states and some with completely undetermined spins are omitted. Between 8 MeV and just above 22 MeV, almost all states with spins greater than 6 are assigned to bands, as well as a few states with spins 6 or less. The first two columns in the table show the energy and spin/parity of each state as determined experimentally [24]. Energies are given to four significant figures here, although generally they are known to greater accuracy. Multiple spin/parity values and brackets indicate uncertainty, or considerable theoretical input. The third column is the spin/parity we have chosen from the experimentally allowed possibilities, to obtain the most convincing rotational bands. Extrapolation from better determined states point to gaps in our bands, each with a definite spin/parity and a narrow energy range, and our choices are made to fill these. We have made 21 choices, so some may not be correct. The fourth column shows the assigned band for the state.

| Energy | $J^P$ | $J^P$ chosen | Band |
|--------|-------|--------------|------|
| 0.0    | 0$^+$ | 0$^+$        | g.s. |
| 3.353  | 0$^+$ | 0$^+$        | A    |
| 3.737  | 3$^-$ | 3$^-$        | g.s. |
| 3.904  | 2$^+$ | 2$^+$        | E    |
| 4.491  | 5$^-$ | 5$^-$        | E    |
| Z     | J^P | J^P' | Decay          |
|-------|-----|------|----------------|
| 5.212 | 0^+ | 0^+  | E²             |
| 5.249 | 2^+ | 2^+  | E²             |
| 5.279 | 4^+ | 4^+  | E/g.s.         |
| 5.614 | 4^- | 4^-  | E              |
| 5.629 | 2^+ | 2^+  | F              |
| 5.903 | 1^- | 1^-  | F              |
| 6.025 | 2^- | 2^-  | E              |
| 6.030 | 3^+ | 3^+  | F              |
| 6.285 | 3^- | 3^-  | A              |
| 6.508 | 4^+ | 4^+  | F              |
| 6.543 | 4^- | 4^-  | E²             |
| 6.582 | 3^- | 3^-  | F              |
| 6.750 | 2^- | 2^-  | E²             |
| 6.909 | 2^+ | 2^+  | A × E          |
| 6.930 | 6^+ | 6^+  | E              |
| 6.931 | 3^- | 3^-  | E²             |
| 6.938 | (1^- to 5^-) | 4^-  | F              |
| 6.950 | 1^- | 1^-  | E × F          |
| 7.100 | (2^+) | 2^+  | E × F          |
| 7.113 | 1^- | 1^-  | A × F          |
| 7.114 | 4^- | 4^-  | E²             |
| 7.239 | (3^-, 4, 5^-) | 5^-  | F              |
| 7.278 | (2, 3)^+ | 3^+  | E × F          |
| 7.301 | 0^+ | 0^+  | A²             |
| 7.307 | (5^+) | 5^+  | E              |
| 7.446 | 3^+, 4^+ | 3^+  | E × F          |
| 7.466 | 2^+ | 2^+  | A × F          |
| 7.532 | 2^- | 2^-  | A × E          |
| 7.561 | 4^+ | 4^+  | E²             |
| 7.623 | (2^-, 3, 4^+) | 4^+  | A              |
| 7.677 | (6^+) | 6^+  | E²             |
| 7.702 | 0^+ | 0^+  | E³             |
| 7.769 | (3, 4, 5^-) | 5^-  | F              |
| 7.815 | 0^+ | 0^+  | A × E²         |
| 7.870 | 3^- | 3^-  | E × F          |
| 7.872 | 2^+ | 2^+  | E³             |
| 7.928 | 4^+ | 4^+  | A × E          |
| 7.972 | (≤ 3)^- | 2^-  | E × F          |
| 7.974 | (6^+) | 6^+  | E²             |
| 7.977 | 2^+ | 2^+  | A × E²         |
| 8.100 | 8^+ | 8^+  | E              |
| 8.135 | (3^-) | 3^-  | E × F          |
| 8.187 | (3, 4, 5^-) | 5^-  | E²             |
| E   | Spin | g.s. | State | Eν | Spin | g.s. | State |
|-----|------|------|-------|----|------|------|-------|
| 8.338 | (2⁺, 3, 4) | 3⁺ | A × F |
| 8.359 | (0, 1, 2⁻) | 0⁻ | E³ |
| 8.364 | (3⁻ to 7⁻) | 3⁻ | A × F |
| 8.374 | 4⁺ | 4⁺ | E × F |
| 8.484 | (1⁻, 2⁻, 3⁻) | 2⁻ | E³ |
| 8.678 | 4⁺ | 4⁺ | E × F |
| 8.701 | (6⁻) | 6⁻ | E |
| 8.764 | 3⁻ | 3⁻ | E³ |
| 8.851 | 6⁻, 7⁻, 8⁻ | 6⁻ | E² |
| 8.936 | (7⁺) | 7⁺ | E |
| 9.032 | 5⁺, 6⁺, 7⁺ | 6⁺ | g.s. |
| 9.033 | (7⁻) | 7⁻ | E |
| 9.246 | (7⁻) | 7⁻ | F |
| 9.305 | (8⁺) | 8⁺ | E |
| 9.429 | (3, 4⁻) | 4⁻ | E × F |
| 9.454 | 3⁻ | 3⁻ | A² |
| 9.811 | (3⁻, 4⁻, 5⁻) | 5⁻ | E × F |
| 9.853 | (8⁺) | 8⁺ | E² |
| 9.860 | 4⁻, 5⁻, 6⁻ | 6⁻ | g.s. |
| 9.869 | 1⁺, 2⁺ | 1⁺ | E × F |
| 9.921 | (3⁻, 4⁻, 5⁻) | 4⁻ | A × E |
| 10.05 | (3⁻ to 7⁻) | 7⁻ | E² |
| 10.15 | (3⁻, 4⁺, 5⁻) | 5⁻ | E × F |
| 10.27 | 3⁺, 4⁺, 5⁺ | 5⁺ | A × E |
| 10.47 | (8⁻) | 8⁻ | E |
| 10.82 | 3⁺ | 3⁺ | E³ |
| 10.89 | (9⁻) | 9⁻ | E |
| 11.00 | (10⁺) | 10⁺ | E |
| 11.37 | (5⁻) | 5⁻ | A × E |
| 11.69 | (10⁺) | 10⁺ | E |
| 11.69 | 7⁻ | 7⁻ | g.s. |
| 11.71 | (9⁺) | 9⁺ | E |
| 12.33 | (10⁺) | 10⁺ | E² |
| 12.59 | (10⁺) | 10⁺ | E² |
| 12.92 | (11⁻) | 11⁻ | E |
| 13.12 | (12⁺) | 12⁺ | E |
| 13.19 | (10⁻) | 10⁻ | E |
| 13.54 | (11⁺) | 11⁺ | E |
| 13.62 | 6⁺ | 6⁺ | A |
| 14.23 | (12⁺) | 12⁺ | E |
| 14.87 | (9⁻) | 9⁻ | g.s. |
| 15.15 | (13⁺) | 13⁺ | E |
Table 2: Energy, spin/parity and rovibrational band assignments for states of Calcium-40.

| Energy (MeV) | Spin/Parity | Band Assignment |
|--------------|-------------|-----------------|
| 15.27        | (12⁺)       | 12⁺ E²          |
| 15.31        | (13⁻)       | 13⁻ E           |
| 15.75        | (12⁺)       | 12⁺ E²          |
| 16.53        | (14⁺)       | 14⁺ E           |
| 16.58        | (13⁺)       | 13⁺ E           |
| 17.70        | (14⁺)       | 14⁺ E           |
| 18.05        | (14⁺)       | 14⁺ E           |
| 18.21        | (15⁻)       | 15⁻ E           |
| 18.50        | (14⁺)       | 14⁺ E²          |
| 18.72        | (14⁺)       | 14⁺ E²          |
| 19.20        | (15⁺)       | 15⁺ E           |
| 20.58        | (16⁺)       | 16⁺ E           |
| 22.06        | (16⁺)       | 16⁺ E²          |

References

[1] J. A. Wheeler, Molecular viewpoints in nuclear structure, *Phys. Rev.* 52 (1937) 1083.
[2] W. Wefelmeier, Ein geometrisches Modell des Atomkerns, *Zeit. f. Phys.* A107 (1937) 332.
[3] L. R. Hafstad and E. Teller, The alpha-particle model of the nucleus, *Phys. Rev.* 54 (1938) 681.
[4] K. Lezuo, Ground state rotational bands in $^{16}$O, $^{40}$Ca and $^{208}$Pb?, *Z. Naturforsch.* 30a (1975) 158.
[5] A. Heusler, Identification of rotating and vibrating tetrahedrons in the heavy nucleus $^{208}$Pb, *Eur. Phys. J.* A53 (2017) 215.
[6] D. M. Dennison, Energy levels of the $^{16}$O nucleus, *Phys. Rev.* 96 (1954) 378.
[7] D. Robson, Evidence for the tetrahedral nature of $^{16}$O, *Phys. Rev. Lett.* 42 (1979) 876.
[8] R. Bijker and F. Iachello, Evidence for tetrahedral symmetry in $^{16}$O, *Phys. Rev. Lett.* 112 (2014) 152501.
[9] C. J. Halcrow, C. King and N. S. Manton, Dynamical $\alpha$-cluster model of $^{16}$O, *Phys. Rev. C95* (2017) 031303(R).
[10] C. J. Halcrow, C. King and N. S. Manton, Oxygen-16 spectrum from tetrahedral vibrations and their rotational excitations, *Int. J. Mod. Phys.* E28 (2019) 1950026.
[11] T. H. R. Skyrme, A non-linear field theory, *Proc. Roy. Soc. Lond.* A260 (1961) 127.

[12] R. A. Battye, N. S. Manton and P. M. Sutcliffe, Skyrmions and the $\alpha$-particle model of nuclei, *Proc. Roy. Soc. Lond.* A463 (2007) 261.

[13] G. Herzberg, *Molecular Spectra and Molecular Structure: II. Infrared and Raman Spectra of Polyatomic Molecules*, Van Nostrand, Princeton NJ, 1945.

[14] D. R. Tilley, H. R. Weller and C. M. Cheves, Energy levels of light nuclei $A = 16 – 17$, *Nucl. Phys.* A564 (1993) 1.

[15] J. Suhonen, *From Nucleons to Nucleus*, Springer, Berlin Heidelberg, 2007.

[16] P. H. C. Lau, unpublished.

[17] P. H. C. Lau and N. S. Manton, Quantization of $T_d$- and $O_h$-symmetric Skyrmions, *Phys. Rev.* D89 (2014) 125012.

[18] N. S. Manton, Lightly Bound Skyrmions, Tetrahedra and Magic Numbers, arXiv:1707.04073 (2017).

[19] C. J. Halcrow, N. S. Manton and J. I. Rawlinson, Quantized Skyrmions from SU(4) Weight Diagrams, *Phys. Rev.* C97 (2018) 034307.

[20] M. Gillard, D. Harland and M. Speight, Skyrmions with low binding energies, *Nucl. Phys.* B895 (2015) 272.

[21] M. Gillard, D. Harland, E. Kirk, B. Maybee and M. Speight, A point particle model of lightly bound Skyrmions, *Nucl. Phys.* B917 (2017) 286.

[22] E. Ideguchi et al., Superdeformation in the doubly magic nucleus $^{40}$Ca, *Phys. Rev. Lett.* 87 (2001) 222501.

[23] S. Torilov et al., Spectroscopy of $^{40}$Ca and negative-parity bands, *Eur. Phys. J.* A19 (2004) 307.

[24] Evaluated Nuclear Structure Data File, https://www.nndc.bnl.gov/ensdf/index.jsp.

[25] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics – Course of Theoretical Physics Vol. 3 (3rd ed.)*, Butterworth-Heinemann, Oxford, 1977.

[26] https://en.wikipedia.org/wiki/Numerical_semigroup.

[27] P. R. Bunker and P. Jensen, Spherical top molecules and the molecular symmetry group, *Mol. Phys.* 97 (1999) 255.