Data Analysis of Low-lying Collective Modes in Even-Even Nuclei

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One way to model the systematics of energy levels in nuclei is by considering quantized collective excitations: the collective model of Bohr and Mottelson. This project investigates such methods by data analysis. Using ordinary least squares regression, we attempt to evaluate three excitation modes: harmonic oscillators, harmonic oscillators with two-body perturbation, and rigid rotators. However, this analysis leads to poor classification of nuclides into distinct excitation modes due to lacking a powerful measure of the goodness of fit of our models. To compensate, an old, simple, but powerful analysis is conducted on the even-even nuclides to classify excitation types: computing the ratio of first few energy levels.

Approach The information from this report is heavily based on chapter 6 of [1]. The inspiration for what to consider in the data analysis is from this chapter, as well as the general scope of the project.

Usage Final report for the course PHY2109: Nuclei

Code Available on GitHub at `https://github.com/ZacharyVernec/nuclei-final-project`

Figures Higher-quality figures are available on the GitHub repository. Furthermore, readers are encouraged to download and run the code to see high-resolution, interactive versions of the plotted data, as well as additional plots not reproduced in this report.

I. BACKGROUND: THE COLLECTIVE MODEL

The collective model of nuclei of Bohr and Mottelson is a macroscopic model for nuclei. It does not consider the constituent nucleon, but instead posits a geometric shape for the entire nucleus, formed from the aggregate nucleon interactions.

Since nuclei are spheroidal, the shape of the nucleus can be expanded into spherical harmonics, which gives deformations from a sphere. These deformations can form quantized excitations, known as collective excitations[2].

Since it is a macroscopic model, the accuracy of the Bohr-Mottelson model must be justified either from a theoretical or an empirical perspective. Some features of the collective model can be derived from the Nilsson model, which takes motions of some valence nucleons directly into account; however, the bulk of the justification for the collective model comes from empirical observations. In fact, a certain portion of nuclear research is devoted to identifying which nuclei (or groups of nuclei) can be properly modelled using the collective model for a certain type of excitation.

II. PROJECT SCOPE

The identification of collective excitations in low-lying energy levels of nuclei comes down to comparing all energy levels of the nuclei to all energy levels of the excitation, as well as considering transition rates, moments of inertia, and other pieces of evidence[3, 4].

In this paper, we focus on only a few key pieces of evidence: at first, we consider the first even energy levels, and later one we restrict our focus specifically to the energy ratio of the first few of those levels. The reason for only considering the first even energy will become clear as we discuss the specific excitation types.

Furthermore, we restrict our focus to low-lying levels for simplicity, and only consider a few collective excitation types.

III. METHODS

To perform the model fitting, we use ordinary least squares.

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The main goodness of fit model in use will be the Coefficient of Determination R^2. This measures the the fraction of variance explained by the model.

However, an important limitation is that it doesn't discriminate between random error and systematic error. This means it is important to analyze the plot of residuals for fit models.

Another important fact to take into account is the degrees of freedom of our model. To be able to compare our goodness of fit across models with different degrees of freedom, we should use the *adjusted* coefficient of determination[5]. This is defined as

$$R^2_{\text{adj}} = \frac{n-1}{n-d-1} R^2$$

where n is the number of samples and d is the number of variables of the model ($d = 0$ for the total sum of squares). This comes from adjusting the variance estimates in the calculation of R^2 by the degrees of freedom ($n - d - 1$ and $n - 1$).

Note that the adjusted R^2 is always smaller than the non-adjusted R^2, as it is only measuring the fraction of variance explained by the model above what should be expected by chance given the number of degrees of freedom in our model.

For the rest of the paper, consider R^2 to always stand in for R^2_{adj}.

Finally, note that we require very high values of R^2, as the random errors from our model should be minimal due to the uncertainties in energy measurements being very low.

IV. MODEL FITTING

In this section, we describe different models for collective excitations, fit them to the energy levels, and analyze the results.

A. Oscillator Excitations

The simplest excitation that can be considered is a harmonic oscillator. Of course, we consider quantized versions of these oscillators, with each quantum of oscillation being a phonon, giving energies

$$\hat{H} = \sum_{\text{mode } \alpha} \hbar\omega_\alpha \left(\hat{n_\alpha} + \frac{1}{2} \right)$$

For $\hat{n_\alpha}$ being the number operator, which counts oscillations in mode α. Note that we are considering different modes as independent, which may be an idealization if we were to consider a microscopic model for the nucleus.

In our framework, the possible modes of the harmonic oscillators correspond to the oscillating term of the multipole expansions, and so they correspond to some $Y_{l,m}$ for $l \geq 0$, $m \in [-m, \ldots, m]$ that is oscillating.

However, we will restrict our attention to quadrupole oscillations ($l = 2$), since other multipoles are not low-lying or are not physically relevant.

For deformations of a spherical nucleus, there is a degeneracy all modes m for a given l, which means we have

$$\hat{H} = \hbar\omega\hat{n}$$

where $\hat{n}$ counts quadrupole oscillations in all m. Note we are now ignoring the zero-point energy since our data for nuclear energy levels sets the ground state energy to 0.

We need to consider what levels are possible for an n-photon system. We use addition of angular momentum, with each phonon carrying $J = 2$. The full range of possible angular momentum that can be formed can be deduced from the m-scheme, which will be described in the appendix for the curious. However, for now we consider that for an n-phonon system, the largest possible total angular momentum possible is $J = 2n$, and there is only one way of forming this state (by having all angular momenta aligned). Furthermore, the lowest $J^+ = 2n^+$ energy level will be from the n-phonon state. Therefore, we consider only the lowest energy levels of even J.

This helps avoiding the problem of "intruder levels": energy levels not corresponding the collective motion in question that nevertheless intersperse themselves, which makes it difficult to tell which level to fit to.

1. *Results*

The R^2 values are high, as can be seen in figure 1, with 68% of values being above 0.928. Note also that there is an extreme outlier (126Pb), but most values have R^3 above 0.94.

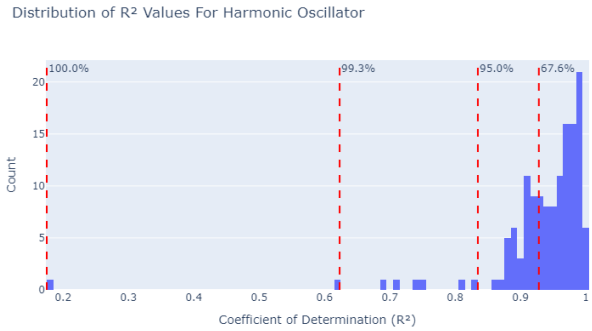
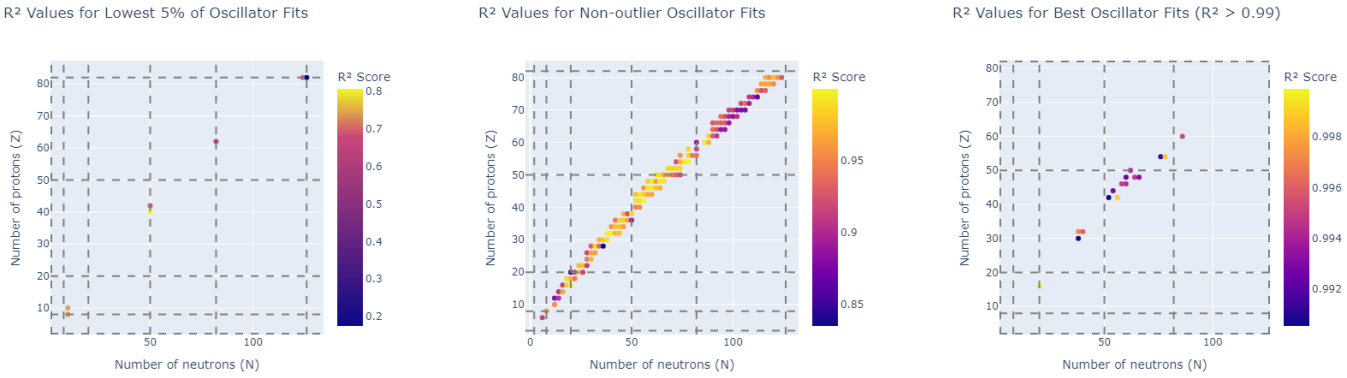


FIG. 1: Histogram of R^2 values for the harmonic oscillator

We can also look at this distribution in the chart of nuclides (fig 2). The 5% worst lie in one of three positions on the chart (figure 2a): along some magic number for heavy nuclei, along one magic number but far from the other for medium nuclei, or are near-magic and light. Now, ignoring the outlier R^2 previously identified, we can investigate which domains fit best (figure 2b). This is difficult to ascertain in general. For $N > 82$, $Z > 58$, the best scores are near magic numbers. For $N \in [30, 82]$, we generally have the best R^2 scores, but no clear pattern relating to the shell model's magic numbers. However, for lighter than ($A < 68$), it gets worse again, with again no clear pattern.

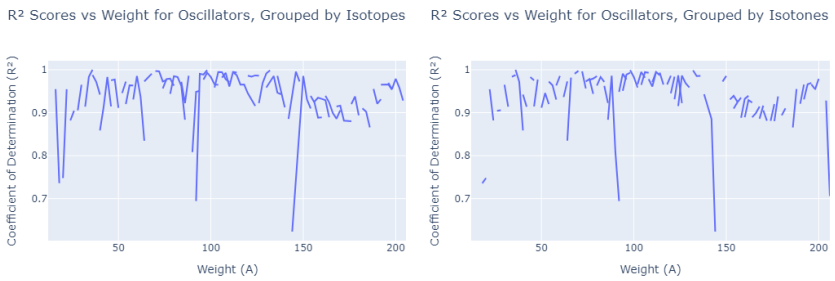


(a) Outlier fits (b) Non-outlier fits (c) Best Fits

FIG. 2: Chart of R^2 values for the Harmonic Oscillator

We can look at isotope or isotone series (figure 3), but again there is no clear pattern to be found The only remark to make is that the worst-fit nuclei are situated at the end of an isotope/isotone series (whether the lightest or heaviest).

Now, we can consider the residuals. Even for the best fits, there are often many systematics being discounted. These systematics can be up to half of a phonon energy, implying that independent phonons are a poor approximation. Alternatively, they may be an indicator that the harmonic oscillator model itself is a poor model for that nuclei. We note that there seem to be some good fits, but also bad fits with residuals in the shape of a U, a sine, or a W (see figure 4 Furthermore, we note that systematic errors often break down or change around some $n \in \{4, 5, 6\}$, especially for residuals of W shape.



(a) Isotope series (b) Isotone series

FIG. 3: Isotope/tone Series for the Harmonic Oscillator

FIG. 4: Residuals of the Harmonic Oscillator Fits with $R^2 > 0.985$, in no particular order. Note that the residuals are normalized to $\hbar\omega$.

B. Oscillators with interactions

One possibility for systematic errors in the harmonic oscillator excitation model may be coming from interactions between phonons. Indeed, in the Nilsson model (and other microscopic perspective model such at the Interacting Boson Model), we note that phonons are formed of particle-hole pairs. The particle and hole in the pairs are fermions, and so the Pauli exclusion principle implies some interaction energy between the pairs. In particular, we assume only two-body interactions.

Suppose the two-phonon interaction energies is δ_2, and let δ_n be the energy shift of n phonons due to two-phonon

interactions. Clearly, $\delta_0 = \delta_1 = 0$ and δ_2 is unknown. For higher number of oscillations, there are $\binom{n}{2}$ ways to create pairs of phonons out of n phonons, so we must have

$$\hat{H} = \hbar\omega\hat{n} + \frac{\delta_2}{2}\hat{n}(\hat{n}-1)$$

Note that our model now has two parameters (the phonon energy $\hbar\omega$ and the two-phonon interaction energy δ_2. This decrement in degrees of freedom of our fit compared to the harmonic-only case justifies our use of the adjusted R^2 measure.

Further note that we must ignore nuclides that only have three levels of data available, as our 2 parameter model would fit it perfectly.

1. *Results*

Despite the adjustment from using more parameters, this model with anharmonicity has much higher R^2 values.

However, we must take note that not all values of δ_2 are permissible in our model. We want δ_2 to be perturbative, that is, for the two-phonon interaction to be much smaller than the phonon energy: $\delta_2 \ll \hbar\omega$. However, if we inspect the distribution o $\delta_2/(\hbar\omega)$ (figure 5), we note that this happens around 17% of the time. There are even two nuclides with shift many multiples of the phonon energy, though these are the same that don't fit well in any model yet: 18O and 20Ne (the lightest even-even nuclides under consideration). Furthermore, many heavy nuclides have a shift of the same order as the phonon energy, even though they had good values of R^2.

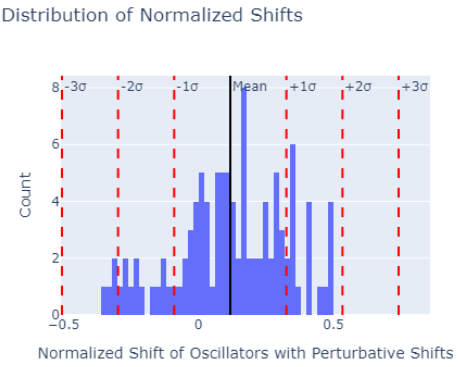


FIG. 5: Distribution of normalized shifts $\delta_2/(\hbar\omega)$ for harmonic oscillators with two-phonon anharmonicity.

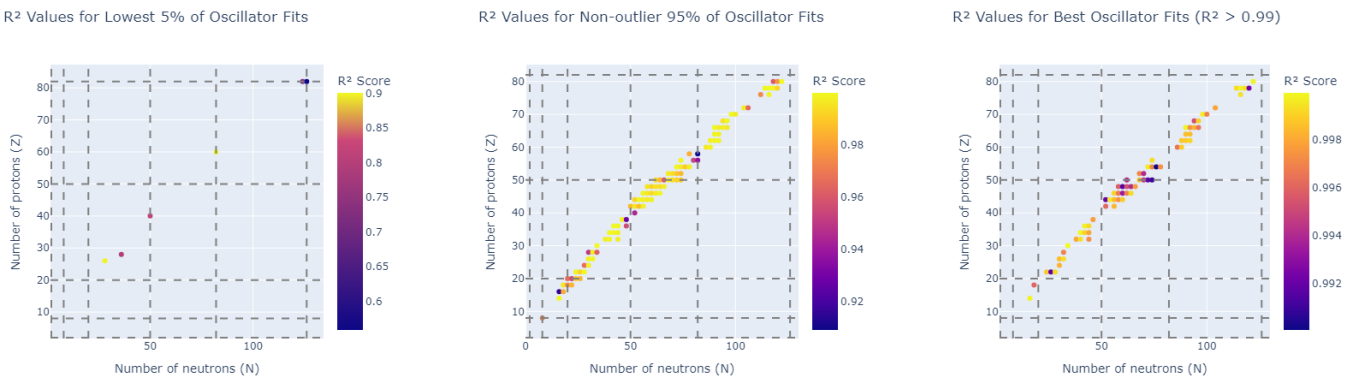
For the remaining analysis, we exclude nuclides such that the fit gives $\delta_2 \geq 0.5\hbar\omega$. Of the remaining, least well fit nuclides are generally the same as the harmonic case (compare figure 6a to figure 2a), though the relative ordering changed slightly to make two switch places across the 5% line. There are much more nuclei with $R^2 > 0.99$, across the whole weight spectrum. Furthermore, when looking at the residual plots for the best fit, we note two points: For one, there are more nuclides in which the systematic error is near-0, i.e. well fit by this model; for two, the residuals can occasionally be on the order of the phonon energy $\hbar\omega$, i.e. the model is still a poor fit.

V. RIGID ROTATORS

Another model to consider is that of the quantum rigid rotator. The Hamiltonian goes as

$$\hat{H} = \frac{\hbar^2}{2I}\hat{L}^2$$

where I is the moment of inertia and $\hat{L}$ is the orbital angular momentum, i.e. the angular momentum of the rotating spheroid[6]. Note that this can only be possible for non-spherical nuclei, as the rotation needs to happen across an axis perpendicular to the axis(axes) of symmetry[1]. The simplest case is when all angular momentum is due to the rigid rotator (i.e. no other sources of angular momentum such as a quadrupole vibration), then we have $\hat{L} = \hat{J}$, and that it can only take even values of J.



(a) Outlier fits (b) Non-outlier fits (c) Best Fits

FIG. 6: Chart of R^2 values for the harmonic oscillator with two-phonon interactions.

A. Results

We can perform the same analysis as before. Unfortunately, we get similar results.

We can test another goodness of fit measure that R^2. We define a new measure RSE/STD as the root squared error (RSE), normalized by the standard deviation of the underlying data (STD). This can be thought of as a measuring how much variance there is in the residuals left after the fit, normalized by the data. However, this measure is not significantly different enough to R^2 to improve results.

VI. NUCLIDE CATEGORIZATION

Finally, we can consider a simple way to categorize the type of first collective oscillation, as long as we assume that the first oscillation is of a collective type (without verifying). The ratio $R = \frac{E_{4+}}{E_{2+}}$ will depend on collective oscillation type.

For a harmonic oscillator, we have

$$R = \frac{\hbar\omega \cdot 2}{\hbar\omega \cdot 1} = 2$$

Considering two-phonon anharmonicities, we have a small shift of $\frac{\delta_2}{\hbar\omega}$. For an axially symmetric rotator, we have

$$R = \frac{\frac{\hbar^2}{2I}4(4+1)}{\frac{\hbar^2}{2I}2(2+1)} = 3.33$$

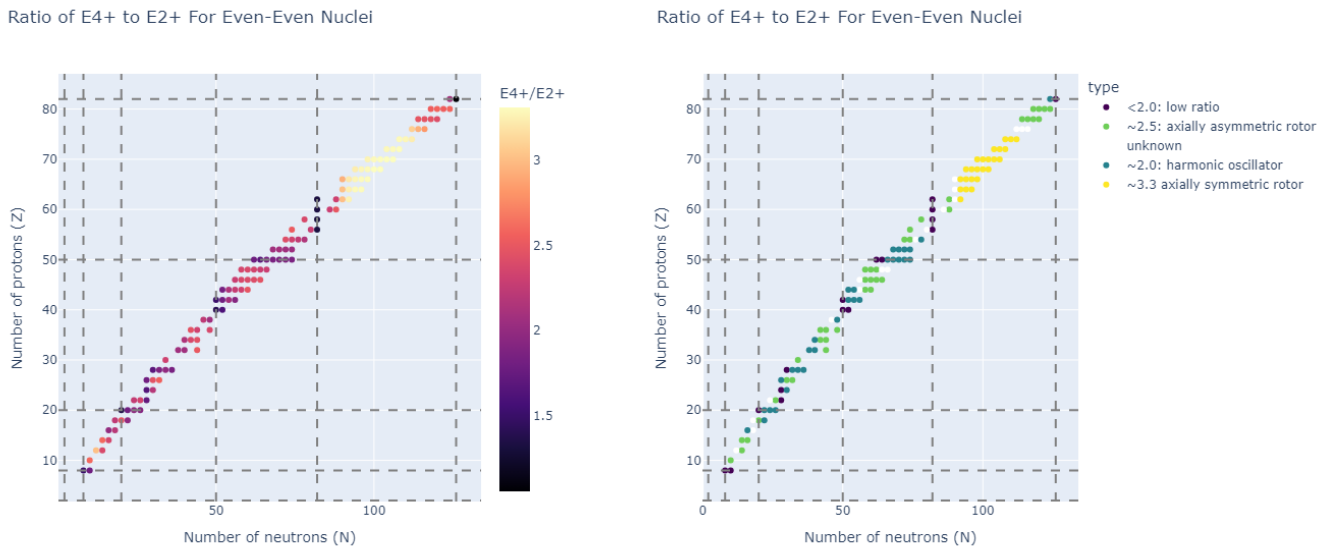
We have not given the Hamiltonian for an axially asymmetric rotator, but according to Casten[1], it would give $R = 2.5$. Furthermore, values of R even lower than a harmonic oscillator are characteristic of filled nuclear shells.

A. Results

We can categorize as such, with a tolerance of 0.2. From figure 7, we can observe patterns. The far-from-magic heavy and medium nuclei are axially symmetric rotators. Doubly magic number nuclides are always with $R < 2$, which is why Casten characterizes them as filled-shell-like energy levels. However, it is important to note that values of $R < 2$ also happen for some singly magic nuclides, even when the other number is far from magic. In fact, singly magic with a near-magic number tend to be harmonic oscillator, especially for light to medium weight nuclides.

VII. FURTHER WORK

There are many places to expand on this basic analysis, without even expanding the scope of the project.



(a) Nuclides chart colored by the continuous values of ratio.

(b) Nuclides chart colored by the category corresponding to their ratio.

FIG. 7: Chart of E_{4^+}/E_{2^+} ratios and their equivalent categorization.

A necessary improvement is to find a measure of goodness of fit that works better than R^2 at telling which models fit well and which don't, that takes into account systematic errors.

A possible expansion of the fit options is to determine, for each model, how many levels fit the model. This is necessary, as it may only be the truly low-lying levels of certain nuclides which are collective excitations, and this cutoff may be different for different nuclides. We have already identified W patterns and sin patters in residuals of some nuclides, showing a possible transition.

It would be nice to correlate the properties of the nuclides to the model fit. In particular, an attempt was briefly made to consider the electric quadrupole moment as a measure of goodness of fit,

An expansion in scope would be to consider more that just the first even levels of nuclides (for example using the m-scheme to find other multi-phonon states), or even to go into other nuclide types such as odd-odd nuclides.

Finally, it would of course be important to compare the results obtained in this data analysis to more meticulous analyses of specific nuclides in the literature, for example in [3].

Appendix A: The m-scheme

The m-scheme consists of first writing out all tuples of m_{J_k} that each particle k may take. Then, for each configuration tuple, calculate the resulting $m_{J_{\text{tot}}} = \sum_k m_{J_k}$ of the system. Finally, note that the largest possible $m_{J_{\text{tot}}}$ must be due to a possible $J_{\text{tot}} = m_{J_{\text{tot}}}$. Take note of this J_{tot}, and for each $m \in [-J_{\text{tot}}, \ldots, J_{\text{tot}}]$, eliminate one configuration tuple giving $m_{J_{\text{tot}}} = m$. Repeat for the largest $m_{J_{\text{tot}}}$ in remaining configuration tuples, until there are no configurations unaccounted for.

Appendix B: Code file organization

- levels.csv is the saved dataset.
- m-scheme.ipynb gives an algorithm to compute the m-scheme.
- project-complicated-oscillator.ipynb is a draft of oscillators with interactions.
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- project-even-even-all-ratio.ipynb does the nuclide categorization
- project-even-even-all.ipynb is a draft attempting to compare goodness of fit across the different models.
- project-even-even-oscillators-adjusted-goodness.ipynb does the same as project-even-even-oscillators-adjusted.ipynb, but with the goodness of fit measure RSE/STD.
- project-even-even-oscillators-adjusted.ipynb does the harmonic oscillator.
- project-even-even-oscillators-anharmonic-perturbative.ipynb does the oscillator with interactions after filtering out for too large phonon interaction energy.
- project-even-even-oscillators-anharmonic.ipynb does the oscillator with interactions for all possible interaction energies, as well as looking at the values of interaction energies.
- project-even-even-rotators-adjusted.ipynb does the rotator model fitting.
- project-even-even-sphericality.ipynb is a draft that attempts to connect the model fits to the electric quadrupole moment as a mesure of non-sphericality.
- project-exploratory.ipynb downloads the initial dataset, as well as doing some draft exploratory analysis.
- project-rotator.ipynb is a draft of the rotators model fitting.
- requirements.txt is the python environment requirements.

Acknowledgments

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