SFU DEPARTMENT OF CHEMISTRY

August 23, 2022

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Prof. Dr. Hab. Ryszard Zdyb
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Dear Prof. Zdyb,

In your letter dated on June, 24, 2022 I was asked to provide a review of the Ph.D. thesis entitled "Systematic study of exotic nuclear shape symmetries and isomers, including shape evolution and competition in Heavy and Super-Heavy Nuclei" authored by Mgr. Jie Yang. In particular, I was asked to evaluate if the thesis fulfills the requirement of Art. 187, Ust. 1, 2, and 3 of the Higher Education Act adopted on July 20, 2018. The Act calls for the PhD thesis to illustrate the knowledge of the Ph.D. candidate in a specific field of study and to provide an evidence that the candidate is capable of pursuing scientific work independently. Moreover, according to the act, the thesis should present an original solution to a scientific question based on the individual studies of the Ph.D. candidate. Following a careful review of the thesis I concluded that the thesis of Mgr. Jie Yang meets all of the above conditions and should be considered as ready for a Ph.D. defence.

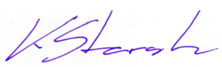
From my personal perspective as a faculty supervising graduate students on a Ph.D. and M.Sc. level I found the thesis as adhering to the highest scientific standards, well organized and carefully considered and planned, well written as well as enjoyable to read and review. I have no doubts that the thesis would be accepted as fulfilling the requirements for a Ph.D. at Simon Fraser University, as well as a number of other universities I had a chance to collaborate in my scientific career. Moreover, it is worth to note here that substantial part of the thesis has been published in a first-author article by Mgr. Jie Yang in Physical Review C (PRC105(2022)034348), one of the highest-impact peer-reviewed journal in the field, which in itself is a best indication of the scientific impact. It is also my understanding that Mgr. Jie Yang is a co-author of multiple other peer-reviewed journals resulting from collaborations with researchers in nuclear theory and experiment. For the above reasons I have no doubt that the thesis should be accepted and that the candidate is ready for a defence. Below I provide a detailed evaluation followed by a list of comments and suggestions for improvements if such can still be implemented.

The scientific concept explored in the thesis, as well as in the PRC article of Mgr. Jie Yang, is the impact of exotic shape distortion, in particular, octupole and hexadecapole deformation, on the structure of atomic nuclei, in particular, heavy nuclei in lead and actinide region. The original contribution, in my view is two-fold. The first comes from a combination of methods from different subfields of theoretical physics and applied mathematics which allow for a large-scale computations of equilibrium shape deformation as a function of excitation energy and rotation frequency throughout a landscape of a few thousand of atomic nuclei. The second comes from the symmetry approach to analysis of results of quantum-mechanical calculations, in particular, to the group-theory driven analysis of predicted shapes and single-particle energy levels. While tools and methods used in the thesis were applied separately in works of other researchers, it is, in my view, the combination of thereof which provide Mgr. Jie Yang with the sensitivity allowing successful extrapolation to the region of heavy nuclei and reliable analysis of signatures of exotic symmetries throughout the nuclear chart. As a result, a new magic octupole quantum number N=136 has been predicted for neutrons in lead and heavier nuclei, while multiple candidates for experimental identification of tetrahedral, octahedral, and shapes representing other exotic point-group symmetries have been proposed. Based on the above I have no doubt that the thesis represents an original solution of a scientific problem presented by Mgr. Jie Yang and provides an excellent evidence indicating that she is capable of independent scientific work of significance.

The part of the thesis which I would consider as presenting the original contribution of Mgr. Jie Yang to the field of nuclear structure is the second part entitled “Results and Discussion”. The first part containing five chapters provides a comprehensive review of the methods used by Mgr. Jie Yang in her research. These chapters include an overview of the open questions in nuclear structure, a review of the nuclear mean-field theory of nuclear structure, a review of methods for solving the Schroedinger equation for the mean-field nuclear Hamiltonian, a review of including residual pairing correlations into the mean-filed calculations, and finally, the review of applications of Group Theory to the analysis of a symmetry of the nuclear shape. The thesis also includes an Annex explaining the founding ideas and applications of the macroscopic-microscopic model for predicting nuclear properties such as equilibrium shapes and deformations. In my view these chapters clearly demonstrate a significant body of knowledge which Mgr. Jie Yang had to master in preparation of her research and which she practised and developed during her studies. These chapters are in general clearly written and easy to follow, which demonstrates in my view deep understanding on a conceptual level. Having said that, it is my duty as a reviewer to provide list of suggestions for improvement and request of clarification, which I include as a follow up of this review.

During my professional career I served as a senior supervisor of four Ph.D. and six M.Sc students, served as a Chair of the Departmental Graduate Study Committee in the Department of Chemistry at Simon Fraser University and have been a part of Supervisory Committees of multiple graduate students. With this perspective I am confident to conclude that the Ph.D. thesis submitted by Mgr. Jie Yang would be in the top 10% of graduate theses I evaluated thus far and would have no problem being accepted at Simon Fraser University or other universities I am familiar with. I have no doubt that the work presented in the thesis is free of any major flows in the methodology and that the results and conclusions are scientifically sound and defensible. The list of comments and suggestion below addresses only minor points and does not impact the conclusions and main findings of the thesis. I would like to stress that the recognition of significance of the work done by Mgr. Jie Yang is not only mine, but had to be supported by anonymous reviewers of the PRC article first-authored by her. In summary, I deemed the thesis as of fulfilling the requirements of the Higher Education Act for awarding a Ph.D. and ready for the defence. If the thesis could qualify for a competition for an award I would be more then happy to provide further support. In case of any further questions, please, do not hesitate to contact me directly.

Sincerely yours,



Krzysztof Starosta

Comments and Suggestions on Mgr. Jie Yang Ph.D. thesis

August 23, 2022

1 Comments on merit of the thesis

- Below 2.1.15 it is stated that nuclear interactions are proportional to certain mathematical operators. I think the correct statement is that the model for interactions is constructed to be proportional to these terms.
- Above Eq. 2.3.1 it should be specified that spherical harmonics are used for expansion of functions dependent on the azimuthal and polar angle in spherical coordinates, not an arbitrary function (for example, an arbitrary function of the radial coordinate can not be expanded into spherical harmonics).
- As far as I understand Eq. 2.3.23 holds when the Condon-Shortly phase is used. At least a comment is needed here to clarify the sign convention used in the thesis.
- I have a hard time to understand Chapter 2.3.4. In particular, I do not see how the surface would be a scalar, it can be easily demonstrated that the formula defining a nuclear surface has to be dependent on the choice of the coordinate system. In particular, Eq. 2.3.27 is not stating the condition for an invariance, but rather for a specific form of variance. Also, there is a statement in the last line of page 85 and the first line of page 86 stating that a symmetric object coincides with itself before and after transformation corresponding to the symmetry, which, in my view is correct but inconsistent with the presentation in Chapter 2.3.4. I think Chapter 2.3.4 needs to be revisited. However, I think the results of this chapter are not used in calculations. This chapter, in my view, can also be eliminated without a consequence.
- Eq. 2.3.27 is inconsistent with the definition of the nuclear surface in Eq. 2.3.1. Consequently Eq. 2.3.28 is developed without maintaining the consistency with Eq. 2.3.1.
- The concept of an intruder orbital is used without an explanation in Chapter 2.4.2.

- Eq. 2.4.4 should be explained or derived to illustrate the consistency and correspondence with Eq. 2.1.7 and 2.1.8. This can be done in an Appendix with a reference to the Appendix added to Chapter 2.4.2.
- In Chapter 2.4.4 derivatives are computed for the use of Newton's method. However, this chapter does not discuss how the method was used and implemented. As is, the derivations presented in Chapter 2.4.4 are inconsequential for the thesis. I think the thesis would benefit from adding comments on implementation and application of the Newton's method in the computations presented in the thesis.
- As far as I see Eq. 2.4.27 is derived under the assumption that there is no monopole and dipole term in Eq.2.3.1. Eq. 2.3.1 does not specify the range for the multipole order λ. This inconsistency should be resolved.
- Chapter 2.4.6 at the end states the need of shifting the position of the centre of mass to remove nonphysical consequences of surface deformation. However, it does not explain how these shifts are implemented. I think an explanation provided here would help the reader.
- Chapter 2.4.7 states that there is a dipole moment when the centre of mass is not positioned at zero. This is inconsistent with the statement made in Chapter 2.4.6 that the centre of mass is maintained to be at zero. I think the dipole moment is present when the centre of charge and the centre of mass are not in the same position. These inconsistencies should be resolved.
- The choice of the weight in Eq. 2.5.7 biases the fits towards high-j intruder orbitals. Why would this choice be beneficial? A measurement of the energy, for example, provides a single value, irrespective of the angular momentum of the orbital being measured. For energy measurement, the degeneracy of an orbital does not lead to an increase in information content proportional to the degeneracy.
- Eq. 2.5.17 specifies the correlation between the radius and the depth of the central potential shown in Fig. 2.5.1. There is no equivalent formula provided for the correlation shown in Fig. 2.5.2. I think it would be better to treat the presentation of the correlations in Fig. 2.5.1 and 2.5.2 on the same footing.
- For the purpose of Eq.2.6.21 I would remind the reader that σ_y^2 is the 2x2 identity matrix.
- I think the statement given at the end of Chapter 2.6.2 that rotational spectra can be classified in terms of the the signature quantum number is valid for the specific case of rotation about a principle axis of the intrinsic coordinate frame but is not valid in general. This should be explained and clarified.

- The statement that nuclear interactions conserve parity as given above Eq. 2.6.35 is specific to the interactions originating from the strong force, the weak force does not conserve parity.

- I think the argument at end of Chapter 2.6.4 shows more than stated on page 39, it shows that $\alpha_{\lambda\mu}$ does not need to be real, the condition of nuclear surface being real is sufficient for the surface to be invariant under the y-simplex operator.

- I do not see how is it possible for the parameter λ^{so} to be dimension-less, as stated below Eq. 3.1.5, since the potential has to have the dimension of energy. This should be clarified.

- In Eq. 3.2.23 in the footnote on page 46, the right hand side is missing implementation of the the limits for the integral specified on the left hand side. Consequently, as given, the equation can not be correct. Also, I am not sure if equations in the footnotes should be labelled as on page 46?

- At the end of Chapter 3.2.3 there is a comment on phase convention related to time reversal for matrix elements of the spin operator. I think a comment would be appropriate specifying explicitly the phase convention selected for the thesis, with a reference to previous Chapters in the thesis discussing the time reversal operator.

- Eq. 3.3.2 is a specific implementation of Eq. 2.6.1 which corresponds to selection of $\eta = 1$. This should be clearly stated.

- I think the derivation presented by Eq. 3.3.7 deserves more explanation. In particular, I would like to see more explanation on the step connecting the left hand side and the right hand side for the equality sign in the middle of the equation with the change of the time reversal operator from acting on the wave functions to acting on the operator $\mathcal{O}$. I think this step is not trivial and it would help to guide the reader further in presentation of this result. Furthermore, as far as I see, Eqs. 3.4.8 and 3.49 are specific cases of Eq. 3.3.7 but I am not sure if there is consistency in derivation of thereof, specifically, in the way the complex conjugations are done. I think it would help to clarify.

- Chapter 4.1.1 uses the formalism of the second quantization without stating that or introducing it.

- As far as I see, Eq. 4.2.21 is contradictory, it states that the result of acting with a creation operator and annihilation operator on a bra states is equal. That can not be true and should be clarified.

- There is a statement above Eq. 4.3.1 that a quantum object can not rotate about its symmetry axis. This is, formally, incorrect, an object can rotate around its symmetry axis, the rotation generates a phase and as a result, such a rotation does not change the state. However, there is nothing preventing anybody from acting with the operator of rotation about the symmetry axis on a wave function which is axially symmetric with respect to that axis.

- Eq. 4.3.11 is valid as long as the changes in energy and in angular momentum originate from a collective rotation. I think the problem which is more significant than using the finite difference here is to apply Eq. 4.3.11 to excitations which are not rotational. For each set of nuclear states energy and angular momentum exists, but not for all of them Eq. 4.3.11 holds. I think a clarifying comment would be helpful.

- A statement of neglecting the $\hat{H}_4$ part of Eq. 4.4.13 comes quite late in Chapter 4.4.2. I think it would help to state that fact earlier to explain why the $\hat{H}_4$ part is not given in Eq. 4.4.15-4.4.16.

- I think Chapter 5.1.3 could benefit from adding a diagram showing classification scheme for point group symmetries, for example as given for molecules in here.

- Eq. 5.2.3 restricts the order of λ to larger than 2 eliminating effectively the monopole and the dipole term. I think this restriction should be introduced at the time when the nuclear surface is defined in Chapter 2.3 and a comment should be added that the monopole term is eliminated through the volume conservation while the dipole term is eliminated through the conservation of the position of the centre of mass (if indeed this is the case, otherwise, the correct explanation should be included).

- I think the discussion at the start of page 104 should include a statement that polynomials in question are constructed from the angular momentum operators $\hat{I}_x$, $\hat{I}_y$, and $\hat{I}_z$.

- I think it would be helpful to explain or provide a reference explaining parity projector operators of Eq. 5.4.7.

- A statement at the end of Chapter 5.4.3 states the proportionality between the energy of a state with spin I and the $I(I+1)$ term. A similar statement is made in the second paragraph starting on page 148, and then again on page 150. I think it would be useful to add a comment why is this the case, and why the extra terms in Eq. 5.4.1 preserve this relationship.

- A statement in the first paragraph of Chapter 6.2.1 defines interactions between the $1j_{15/2}$ $N = 7$ orbital and the $2g_{9/2}$ $N = 6$ orbital as repulsive. A similar statement is made at the start of Chapter 6.3. I think a comment explaining why is this the case would be helpful. If this is the statement of non-crossing of quantum levels I think the interactions being repulsive or attractive does not play a role in a two-level mixing model since the energy gap depends on the modulus square of the matrix element.

- I think Chapters 6.2.2 and 6.4 discussing the octupole effects in heavy lead isotopes would benefit from including an argument explaining the origin of the low-lying positive parity states in ^{210}Pb, ^{212}Pb and possibly other lead isotopes in the vicinity of ^{208}Pb. The data, for example posted on the NNDC, indicates that there are multiple states of positive parity below the lowest negative-parity 3^- state located at the energy of about 1900 keV. These positive parity states show the patterns characteristic to single-particle multiplets of two nucleons in the same orbital, which actually is an argument supporting lack of collective quadrupole excitations, consistent with the result presented in the thesis. Without this argument an incorrect argument can be made for the presence of quadrupole excitations based on a comparison of the energy of the first-excited 2^+ state which is about 800 keV to the energy of the first excited 3^- state. Incorrectness of such argument can be demonstrated by pointing out that the 2^+ state does not originate from collective excitations but rather from single-particle excitations.

- The discussion presented in Chapter 6.4.4 does not explain what are the consequences of connecting minima using Dijkstra algorithm. In particular, I understand that the algorithm is finding the shortest path between two minima. However, it is unclear to me what are the consequences of this path being found. The path exists, is found, and it would seem natural to explain how does the identification of the path influences results presented in the thesis.

- I do not understand why the probability densities presented in Fig. 6.5.1, 6.5.2, and 6.5.3 are not symmetric with respect to the centre of the potential (located at the deformation of zero). I think they should be as long as the minima are of equal depth. Is this effect correct or an artifact of the way the equations were solved?

- Energies quoted at the end of the first paragraph on page 166 should be given using units. If some arbitrary units are used that should be stated.

- Eq. 6.7.5 is the first order approximation for an axially symmetric shape which should be stated.

- At the end of the first paragraph of Chapter 6.8.2 it is stated that the linear combination of spherical harmonics with $\lambda = 3$ and $\mu = 0, 2$ is equivalent to that of $\mu = 3$. I think an explanation is needed, since taking into account orthogonality of spherical harmonics one would think that the modes should be independent.

- I think Chapter 8.1 should explain that the macroscopic part of the energy in Eq. 8.1.1 varies slowly as a function of the mass and the atomic number, in contrast to the microscopic part which may vary quite rapidly.

- In Sec. 8.1.1 it is stated in the second line that the liquid drop model has been used to model the energy as a function of deformation. I think the primary role is to model the energy as a function of the mass and the atomic number, not deformation.

- Definitions 8.1.3 and 8.1.4 are inconsistent. Specifically, 8.1.3 resembles the definition of the binding energy, while 8.1.4 is the definition of the mass, not energy. Also, for the second bullet point below Eq. 8.1.3 the contribution of the surface term to the binding energy is repulsive not attracting, since it results from the lack of attracting volume interactions on the surface.

2 Comments on the presentation style in the thesis

2.1 Formatting

- Page numbering is inconsistent, page numbering is restarted in Chapter 1. As a consequence pages 1, 2 and 3 appear two times, first in the Abstract, then in the Introduction.
- As far as I see, the first cited reference is Ref. 5 cited below Eq. 2.1.3. References 1-4 are listed in the "List of Figures". I am not sure what the required convention is, but most often the references should be cited in order of citations, and figures in the list are cited in the text later than Ref. 5 in Chapter 2.
- The axes of reference frames in Fig. 4.3.3 do not look orthogonal. I think the figure can be improved in that sense.
- I think the statement in the last line above the footnote on page 94 should read "... the 3 solutions for the lowest λ", to drive the point across.
- According to the caption of Fig. 5.3.2 there should be dashed lines representing some of the representations of the symmetry groups but the dashed lines are not visible in my copy of the thesis.
- Caption of Tab. 6.3.1 makes a reference to the Annex "Groups", while there is no Annex entitled "Groups" in the thesis.
- I would call Chapter 8 "Appendix" not "Annex".

2.2 Use of mathematical symbols

- Eq. 2.1.8 uses $\wedge$ as a symbol of the cross product for vectors. Similarly the symbol $\times$ is used for a product of operators in Eq. 3.3.18. These should be explained as a convention adopted in the thesis and used in a consistent way. Observe that some equations, for example 5.1.20, do not use a symbol for a product of operators, while other equations, for example the one below 5.1.9 on page 86 use $\circ$, while some other, for example 5.3.1

use $\cdot$. I think defining the conventions and consistency would help the presentation.

- Eq. 2.1.9 should use V_{LL^2} instead of V_{LL} for the term on the left-hand side and the first term on the right-hand side to maintain consistency with Eq. 2.1.3.
- The symbol for a kinetic energy operator for a single particle used in Eq. 2.2.9 is not consistent with the symbol used in Eq. 2.2.3.
- The symbol for a single particle wave function used in Eqs. 2.2.9, 2.5.4, and 3.1.1, is not consistent with the symbol used for a single-particle wave function in Eq. 2.2.6.
- The Greek symbol ψ used to denote a single-particle wave function in Eq. 2.2.9 was used to denote a many-body wave function in Eq. 2.2.6.
- Greek symbol Σ used in Eq. 2.3.1 to denote the nuclear surface was used in Chapter 2.1 to denote a reference frame.
- Below Eq.2.4.11 explain that N_θ and N_ϕ denote partial derivatives of $N(\theta,\phi)$ with respect to θ and ϕ.
- In Eq. 2.4.15 and 2.4.16 the symbols representing partial derivatives of the R function should be explained.
- Symbol $\mathcal{O}_z$ is used below Eq. 2.4.24 to denote the z axis. I understand that this has been done for consistency with the description of symmetries in later chapters, but an explanation or a statement of thereof would help the reader in my view.
- Symbol $\hat{\pi}$ used for the inversion operator in Eq. 2.6.37 is inconsistent with Eq. 2.6.32.
- I would suggest to start Eq. 2.6.45 as $\alpha_{\lambda\mu}Y_{\lambda\mu}(\theta,\phi) + \alpha^*_{\lambda\mu}Y^*_{\lambda\mu}(\theta,\phi) =$
- Eq. 3.3.19 is incorrect, the rotation operator changes signs of the coordinates x, y and z, but is presented as changing the order of Hermite polynomials n_x, n_y and n_z. The order of Hermite polynomials is non-negative.
- The first symbol for the rotation operator on the right hand side of Eq. 3.3.20 is missing the y subscript. Also, as far as I see, this equation is derived incorrectly, since the change of sign in the second line comes from the spin term at the very end of the second line and should not be incorporated into the $(-i^{n_y})$ term. The third line is correct, but the second line is not.

- I think equation 4.1.5 is incorrectly developed for the time reversal part, in particular, the time reversal operator should act on each wave function individually. I think the final result is correct, the presentation could be more rigorous.
- In Chapter 4.4 symbol α is used to denote quasiparticle creation and annihilation operators, for example in Eq. 4.4.8, but also as a summation index in Eq. 4.4.13-4.4.22. I think this may, potentially lead to confusion.
- Eq. 5.1.13 uses a wrong symbol for a product of rotation operators o instead of $\circ$.
- The order of operators in Eq. 5.1.20 is inconsistent with the description of the order given above the equation.
- I think Eq. 5.3.4 is missing the symbol for a sum over the index j, and in a similar way, Eq. 5.3.5 is missing symbols for sums over indices j and k, and further, the right hand side of Eq. 5.3.6 is missing the symbol for a sum over the index i. If Einstein's summation convention is used that should be stated, though, the convention should then be used systematically in the whole thesis, which, as far as I see, is not the case.
- The symbol for basis states v_i used in the sentence above Eq. 5.3.6 is inconsistent with a symbol used in Eqs. 5.3.4 and 5.3.5. I think the change of the symbol is not necessary, and if it is necessary there should be a comment explaining the reason.
- It is said below Eq. 5.4.5 that the symbol C_i denotes the inversion group. I think this should be clarified, since, I think this symbol is used to denote the representation of the inversion group, not the group. Also, a similar symbol was used already to denote a discrete rotation group, see Eq. 5.1.18. I think the thesis would benefit if a possible confusion here is avoided.
- The deformations discussed in the last paragraph on page 168 should be specified in terms of the α_{32} or α_{30} symbols to drive the argument across.

2.3 Language style or spelling errors in English

I am listing errors which I noticed, examining the correctness of the language was not the first priority in the review of the thesis. Consequently, there may be style or spelling errors I missed.

- Page 1 of the Introduction, line 10 from the bottom, "allowing nuclear experimentalists" rather than "allowing to the nuclear experimentalists"
- Page 2 of the Introduction, the top line "on one hand" instead of "on the one hand"

- Page 12, second line from the top “moving with respect” instead of “moving respect”.
- Page 13, fourth line from the top “complex many body-system” instead of “complex in many body-system”.
- Page 24 three lines below Eq. 2.4.37 “the position of origin” rather than “the original position”.
- I would not use the term “image” in reference to wave functions above Eq. 2.6.7 and 2.6.13, I would use the term “wave function”.
- Above Eq.2.6.40 “symmetric with respect to inversion and signature” instead of “obeying to the inversion and signature symmetries”.
- I think the solutions of the Schroedinger equation for a harmonic oscillator are called “Hermite polynomials” not “Hermit polynomials”. The name “Hermit” is used on page 41 third line of the second paragraph, on page 44 above Eq. 3.2.6, in Chapter 3.2.2, but also in numerous other places in the thesis.
- In the first sentence of Chapter 4.1.1 “results regarding” instead of “results about”.
- In the forth sentence of “Basic Ideas” in Chapter 4.2 “create pairs” instead of “create couples”. Also, three lines down “impose an approximate conservation” instead of “assure and approximate conservation”.
- In the caption of Fig. 4.3.1, “denoted” instead of “demoted”.
- The term “The minimum precision” used in line 7 on page 85 is unclear. I think the meaning should be “The minimal set of definitions”. The last sentence of the first paragraph on page 85 should be rephrased to clarify the meaning.
- The statement four lines below Eq. 5.2.1 should read “are larger the higher the order of λ” and does not require repetitions which are used.
- I would suggest “expected” instead of “privileged” in the fifth line of Sec. 5.4.
- I would suggest “rate” instead of “speed” in the second line on page 141.
- Two lines above the start of Chapter 6.4.3 I would suggest “branch” instead of “chapter” and also removing “the” ahead of “Group Theory”.
- On page 190 at the bottom I would suggest “Synthesis ... took place ...” instead of “Synthesis ... was produced ...”
- In the forth line of the third paragraph on page 198 “... we compare the proton ...” instead of “... we compare of the proton ...”.

2.4 Spelling errors in Polish

First, I would gladly admit as a Pole, that Polish spelling is some kind of curse inflicted on the mankind. Having said that

- Page 2 before the Introduction, line 6 from the bottom “Przedstawiliśmy” instead of “Przedsawiliśmy”.
- Page 3 before the Introduction, line 1 from the top “ciężkich” instead of “cieężkich”.

These are the only two I found, thus congratulations on the job well done!