Describing Quadrupole Collective Excitations of Nuclei within Self-Consistent Methods

A link between microscopic HFB calculations and the Bohr Hamiltonian

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Introduction
Awarded “for the discovery of the connection between collective motion and particle motion in atomic nuclei and the development of the theory of the structure of the atomic nucleus based on this connection”.

1See https://www.nobelprize.org/nobel_prizes/physics/laureates/1975/index.html
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- Systematic study of the nuclear chart.
  - Skyrme functional (UNEDF0)
  - Explore isotopic trends in the Rare-Earth region
  - Systematic study of the first low-lying $0^+_1$ state
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PhD Project

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- Provide theoretical support to nuclear experiment.
- Enable using information on collective states for the adjustments of coupling constants of new novel density functionals.
Background Theory
Even-Even Nuclei

\[ Z: 50 - 82 \]

\[ N: 82 - 126 \]

Long isotopic chains to compare to experiment.

Region to predict.

Given the nature of the project \textbf{DFT} is the most appropriate choice.
The Bohr Hamiltonian

In order to describe the collective motion of nucleons we require a collective Hamiltonian\(^2\) given by

\[ \hat{H}_{\text{coll}} = \hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + \hat{V}(\beta, \gamma). \]

- 5 dimensional Hamiltonian
- Expressed in terms of \(\beta\gamma\) deformation parameters
- Input mass parameters (\(\{B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\beta}, B_{\gamma\gamma}\}\) and \(\{B_x, B_y, B_z\}\)) calculated microscopically
- Beyond mean-field calculation

What can we Calculate?

Theoretical Calculations:
- Potential Energy Surfaces
- Mass Parameters and Moments of Inertia
- Pairing Gaps/Pairing Energy

Observables:
- Energy Spectra
- $B(E2)$ Transition Probabilities
Results
Collaborations:

1. $^{94}$Zr, $^{96}$Zr, $^{72}$Se, $^{74}$Se - in progress.
   - Dan Doherty (University of Surrey)

2. $^{80}$Zr, $^{76}$Sr, $^{78}$Sr, $^{72}$Kr, $^{68}$Se - in progress.
   - Ryan Llewellyn (University of York)
   - Jesus Pereira-Lopez (University of York)
   - Bob Wadsworth (University of York)
   - Mike Bentley (University of York)

3. $^{12}$C - in progress.
   - Juan Saiz Lomas (University of York)
   - Marina Petri (University of York)

Further collaborations are most welcome - please feel free to contact me.
The general trend of the isotopic chain is reproduced well. Discrepancies exist immediately following the semi-magic nucleus $^{90}$Zr.

**Figure 2:** Energy of the first $2_1^+$ and first $4_1^+$ states of the Zirconium (Zr) isotopic chain.
The general structure of the spectra is reproduced well.

The Thouless-Valatin scaling can (in some cases) be adjusted until good agreement with experiment is reached.

**Figure 3:** Energy states of the Zirconium-80 ($^{80}$Zr) (unscaled blue, scaling of 1.3 in red and scaling of 1.2 in green).
The structure (ordering) of the states is reproduced reasonably well for both functionals.

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**Figure 4:** States for $^{126}$Xe for both the UNEDF0 and UNEDF1SO functionals with and without the Thouless-Valatin correction (scaling of 30%)$^3$.

Most nuclei have at least one NEDF which lies within the experimental error bars.

**Figure 5:** $B\left(E2 : 2^+_1 \rightarrow 0^+_1\right)$ transition probabilities for a selection of $N = Z$ nuclei.
The majority of nuclei lie within ±200 keV of the experimental value.

Figure 6: $2^+_1$ (left) and $4^+_1$ (right) nuclear energy states absolute error.
Future Work
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- Examine the functional dependency.
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- Explore the role pairing plays in this formalism.
- Calculate a theoretical error for the results using error propagation.
- Expand the current procedure to describe odd nuclei.
- Incorporate octupole and hexadecapole deformations.
- Explore the potential of carrying out a full Adiabatic Time-Dependent Hartree-Fock-Bogoliubov (ATDHFB) calculation.
Collaborators

Thanks to all of my collaborators:

- Leszek Próchniak
- Alessandro Pastore
- Jacek Dobaczewski
THANK YOU FOR YOUR ATTENTION. ANY QUESTIONS OR COMMENTS?

Any suggestions regarding the current work or the future development of this research is most welcome.