Projected mean-fields for isotope shifts

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Introduction

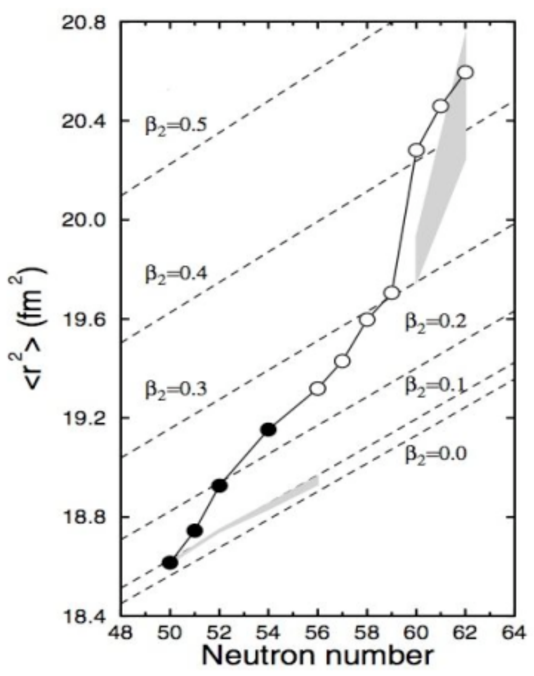
The systematics of nuclear shapes and sizes in the neutron-rich region around A~100 is of long-standing interest due to several characteristic features that have been observed from optical measurements across isotopic chains.

In order to obtain a better understanding of the features in this region of the nuclear chart it is necessary to be able to describe them using theoretical models. This may be achieved through studies within the framework of axially-deformed projected mean-field calculations[1].

Experimental Motivation

Recent experimental data on mean-square charge radii spanning the N=50 shell closure across the Zirconium isotopes show a sharp increase at N=60, creating a discontinuity in an otherwise steadily increasing function as one approaches the neutron drip-line[2]. This is thought to be due to a shape change, which is characteristic of the features of nuclei in this region.

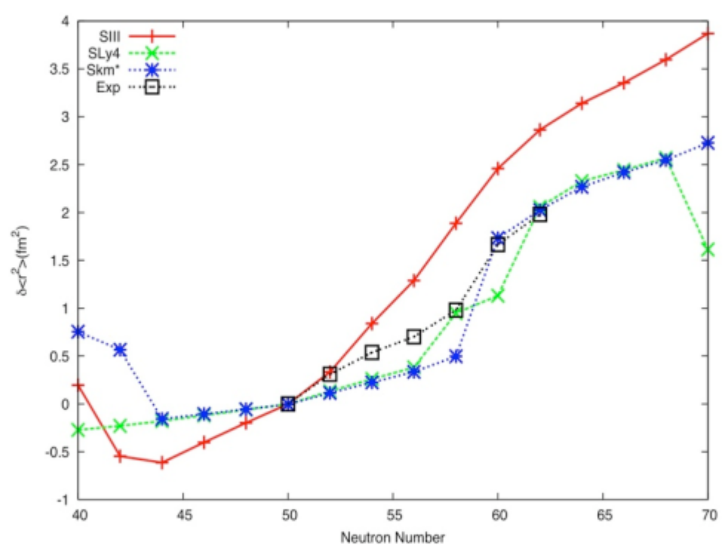
If $\delta\langle r^2\rangle$ are attributed solely to changes in the static quadrupole deformation values, the observations are well reproduced in regions of strong deformation (N≥60). However, this assumption alone fails to explain the observed trends in the transitional region (N<58). A gradual increase in deformation throughout this region is suggested, which infers a significant contribution from dynamical deformations.



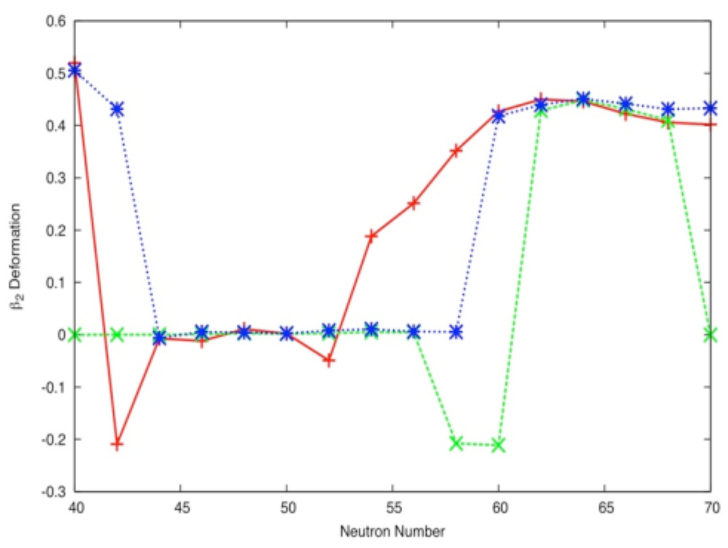
Zirconium mean-square charge radii as a function of neutron number

Hartree-Fock Calculations

Theoretical predictions of the ground state deformation and charge radii for these nuclei vary in their ability to model the discontinuity. Axially-deformed Skyrme Hartree-Fock + BCS calculations are, on the whole, able to reproduce the general trends in $\langle r^2\rangle$ across the isotopic chains, successfully modelling the deformed region beyond the discontinuity. However, none of the available Skyrme parameterizations are able to correctly predict the features of the transitional region.



Calculated change in mean-square charge radius for the Zirconium isotopes (with respect to ^{90}Zr)



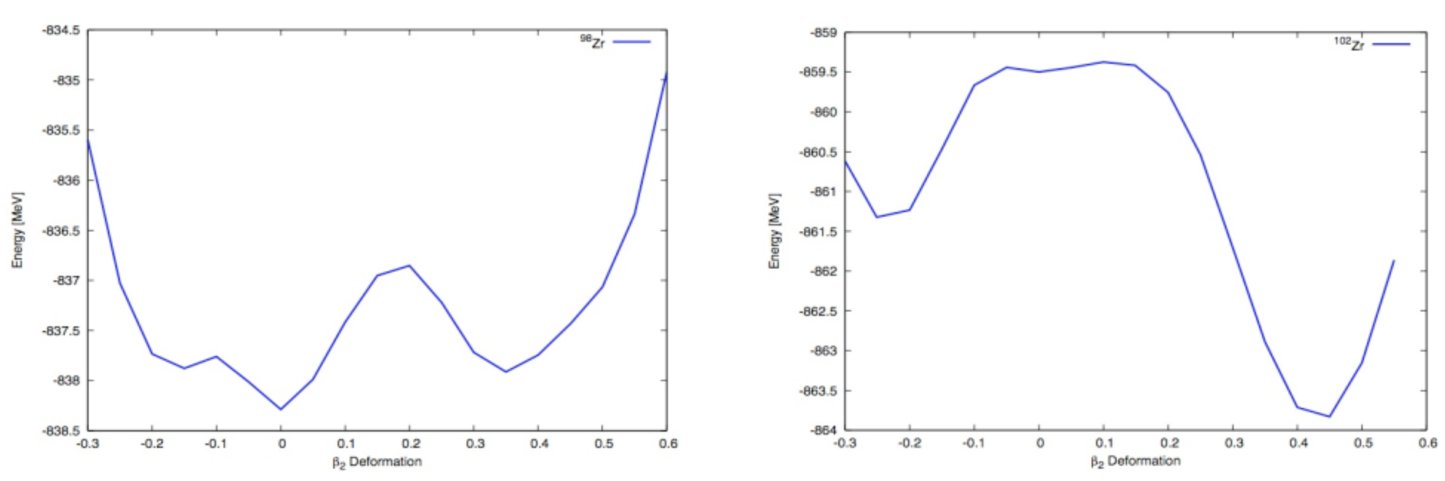
Calculated quadrupole deformation values for the Zirconium isotopes

To explain these discrepancies and better reproduce the overall characteristics of this region it may be necessary to use beyond mean-field techniques such as particle number and angular momentum projection, since the discontinuity is known to occur in a region of softness with respect to shape fluctuations.

Beyond Mean-Field Techniques

One drawback to the HF +BCS prescription is that an uncertainty is introduced in the particle number and total angular momentum. This is due to the fact that the trial wavefunction used in the variational procedure to describe the properties of a particular nucleus is not an eigenstate of these operators. Particle number and angular momentum are therefore not conserved quantities.

In regions of shape 'softness' where there is no clear minimum in the potential energy surface as a function of quadrupole deformation, or the location of the energy minimum changes rapidly with particle number, the state mixing effect could have significant consequences for the calculated properties of these nuclei.



Calculated potential energy surfaces for ^{98}Zr and ^{102}Zr using the SkM Skyrme parameterization. a) Nuclei in the transitional region exhibit softness with respect to shape fluctuations. b) Beyond the discontinuity in mean-square charge radius nuclei are shown to be strongly deformed.*

The broken symmetries associated with mixed states may be restored through particle number and angular momentum projection techniques.

Particle Number Projection

Particle number projection after variation will be performed with respect to the mean-field states following the Fomenko formalism[3]. The basis of the technique is to project out, or extract the 'physical' component of the wavefunction (with BCS form), which is a superposition of states of several neighbouring nuclei. A complex multiplier is applied to the BCS state, which serves to exclude non-physical components without affecting those with good particle number, $2P$, or $P\pm 2l(n+1)$ particles:

$$|\psi_n\rangle = c\left[\prod_{\upsilon}(u_\upsilon + v_\upsilon a_\upsilon^+ a_{-\upsilon}^+) + (-)^P \prod_{\upsilon}(u_\upsilon - v_\upsilon a_\upsilon^+ a_{-\upsilon}^+) + \left\{\sum_{k=1}^{n} e^{-i\pi kP/(n+1)} \prod_{\upsilon}(u_\upsilon + e^{i\pi k/(n+1)} v_\upsilon a_\upsilon^+ a_{-\upsilon}^+) + c.c.\right\}\right]|0\rangle$$

The choice of n reflects the amount of admixture of non-physical components, where their amplitude decreases rapidly away from $2P$ particles.

An expression for the projected energy of the system in terms of the occupation probabilities of single-particle states is obtained by calculating matrix elements in the quasi-particle representation. Initial calculations have been performed for three simple model systems, reproducing the results of Fomenko.

	Exact	BCS	Fomenko (n-value) 0	1	2	3
P-R[4]	6.828	8.082	4.240	6.850	---	---
P=4[5]	13.390	14.972	14.850	13.590	13.560	---
P=8[5]	61.598	64.174	64.097	62.490	62.283	62.282

Calculated ground state energies for three simple models of equally spaced doubly degenerate levels containing 2P particles

Similar expressions for the matrix elements of arbitrary operators may also be calculated using this method, where the effect of restoring the broken symmetry associated with particle number in the mean-field states will be studied directly in terms of charge radius.

Outlook

Beyond mean-field techniques, in particular angular momentum projection, will continue to be developed within the framework of axially-deformed Skyrme HF + BCS models and applied to the A~100 region in attempt to better understand and reproduce their features.

References

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Acknowledgements

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