Density functional theory for exotic nuclear structures

Low Energy RI Science Workshop, July 2022

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Overview

Introduction

Deformed relativistic Hartree Bogoliubov Theory in Continuum (DRHBc)

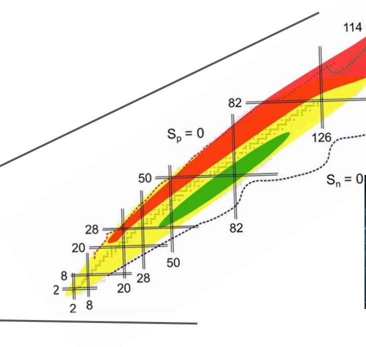
- Description
- DRHBc Mass Table
- Exotic structures in the Oxygen-Calcium region

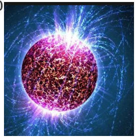
Summary

Introduction

Density Functional Theory

Applicable to the **whole nuclear chart**





Energy of system (nucleus): a functional of the density, E[ρ] (*theorems*)

We do not know the precise form of the functional; **we derive it** using various physical assumptions and strategies

- Non relativistic: Skyrme, Gogny, KIDS
- **Relativistic**
- The variety is useful for cross checks of predictions and for a broader understanding of observed phenomena

Activities at IBS/RISP

Introduction

New *KIDS* on the block

Korea

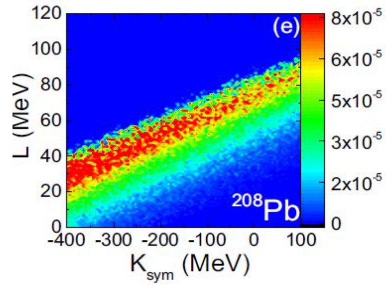
IBS

Daegu

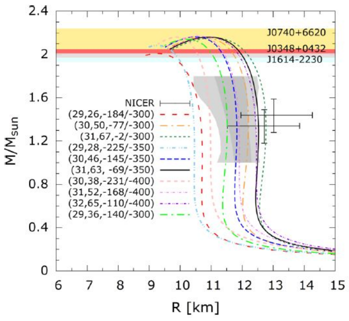
SSKU

Born in 2016 and thriving

- Versatile framework for
  - the nuclear equation of state
  - nuclear structure
  - nuclear response
- Recent investigations: Constraining the symmetry energy parameters from nucelar data and astronomical observations



PHYSICAL REVIEW C **105**, 044305 (2022)

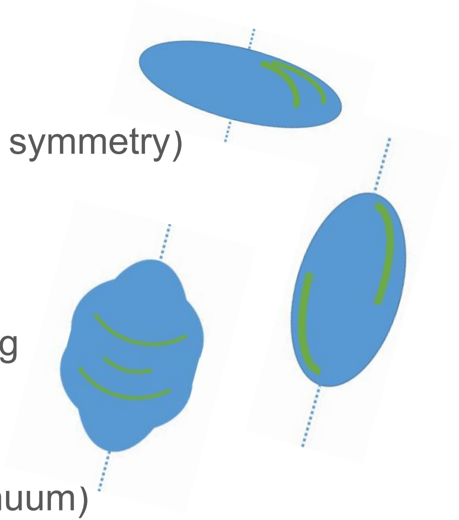


PHYSICAL REVIEW C **103**, 034330 (2021)

Deformed relativistic Hartree Bogoliubov theory in continuum (DRHBc)

Features capabilities which are essential for the description of exotic nuclei

- **Deformation**
  - *Why*: The majority of nuclei are not spherical
  - *How*: Densities and fields are expanded in Lagrange polynomials (axial symmetry)
  - *Bonus*: Beyond quadrupole (oval) shapes
- **Pairing correlations**
  - *Why*: The majority of nuclei do not have closed shells
  - *How*: Density-dependent zero-range pairing force adjusted to staggering
- **Continuum states**
  - *Why*: Drip line nuclei are very close to the continuum (losely bound)
  - *How*: The nuclear mean field is placed in a large box (discretized continuum)



Computational code mainly developed by Chinese colleagues; broad collaboration including Korean teams test and use the code in various studies

DRHBc Mass Table Collaboration

About 50 people

A broad collaboration among several Chinese and Korean teams

Main goal: A complete mass table based on DRHBc

Masses, radii, deformation parameters, nucleon/alpha separation energies

2019-2020: Tests of numerical code for even-even nuclei

2020-2022: Mass Table calculations for even-even nuclei

2021-2022: Code extension to odd nuclei

2022- : Mass table calculations for even-odd nuclei

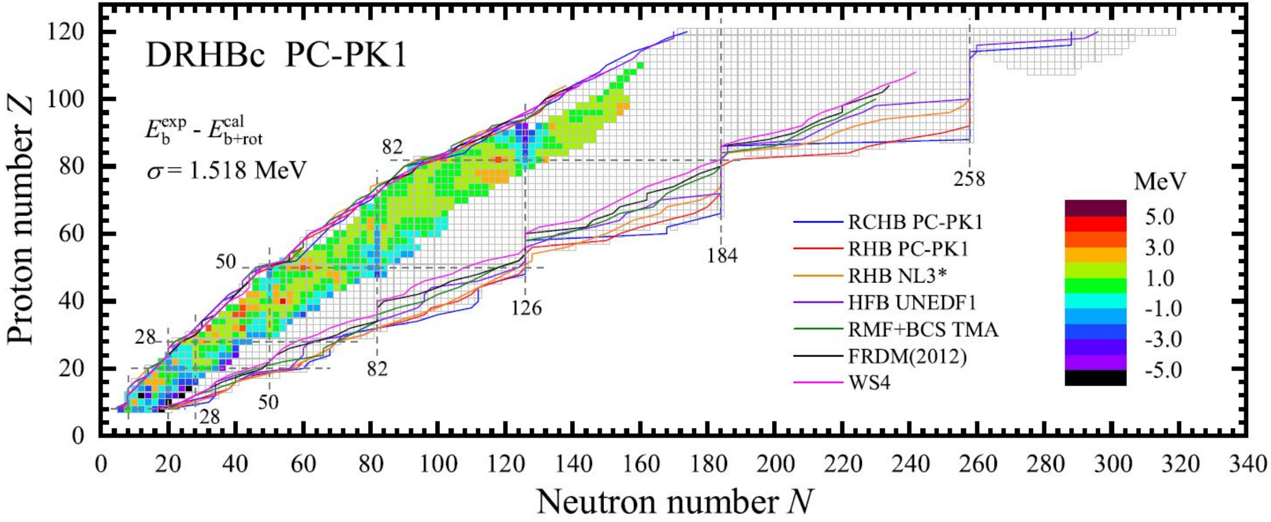
First part: even-even nuclei

Table 1
Ground-state properties.

A	N	E_b^{cal} (MeV)	E_{b+rot}^{cal} (MeV)	E_b^{exp} (MeV)	S_{2n} (MeV)	S_{2p} (MeV)	R_n (fm)	R_p (fm)	R_m (fm)	R_{ch}^{cal} (fm)	R_{ch}^{exp} (fm)	β_{2n}	β_{2p}	β_2	λ_n (MeV)	λ_p (MeV)
$Z = 8$ (O)																
12	4	59.70	59.70	58.58		−2.37	2.329	2.915	2.734	3.022		0.000	0.000	0.000	−19.36	−2.15
14	6	101.16	101.16	98.73	41.46	1.49	2.250	2.639	2.480	2.758		0.000	0.000	0.000	−16.55	−1.18
16	8	127.28	127.28	127.62	26.11	20.45	2.626	2.650	2.638	2.768	2.699	0.000	0.000	0.000	−11.42	−7.78
18	10	140.97	140.97	139.81	13.69	27.18	2.806	2.642	2.734	2.760	2.773	0.000	0.000	0.000	−6.67	−11.63
20	12	152.43	152.43	151.37	11.47	33.79	2.960	2.645	2.838	2.763		0.000	0.000	0.000	−5.70	−15.15
22	14	162.45	162.45	162.03	10.02	40.10	3.105	2.653	2.949	2.771		0.000	0.000	0.000	−4.88	−18.31
24	16	171.07	171.07	168.95	8.62	45.83	3.267	2.659	3.078	2.777		0.000	0.000	0.000	−3.33	−20.24
26	18	174.80	174.80	168.93	3.73	50.72	3.432	2.731	3.232	2.846		0.000	0.000	0.000	−2.12	−22.16
28	20	178.14	178.14		3.34	54.80	3.573	2.794	3.369	2.906		0.000	0.000	0.000	−0.85	−24.13
30	22	177.41	177.41		−0.73	55.27	3.883	2.807	3.627	2.919		0.000	0.000	0.000	0.04	−24.59
σ		2.47	2.47							0.049						
$Z = 10$ (Ne)																
16	6	100.15	100.15	97.33		−1.01	2.286	3.015	2.764	3.119		0.000	0.000	0.000	−19.51	0.50
18	8	133.09	133.09	132.14	32.94	5.81	2.628	2.851	2.754	2.961	2.971	0.000	0.000	0.000	−15.21	−2.47
20	10	155.57	158.24	160.64	22.48	14.60	2.869	2.899	2.884	3.007	3.006	0.535	0.550	0.542	−11.69	−7.47
22	12	175.57	178.50	177.77	20.00	23.13	2.957	2.844	2.906	2.955	2.953	0.494	0.460	0.479	−8.45	−11.51
24	14	189.95	192.86	191.84	14.38	27.50	3.019	2.786	2.924	2.899	2.901	−0.245	−0.197	−0.225	−7.28	−13.05
26	16	201.96	201.96	201.55	12.01	30.89	3.170	2.787	3.029	2.899	2.925	0.000	0.000	0.000	−5.29	−14.50
28	18	209.59	209.59	206.87	7.63	34.79	3.326	2.859	3.167	2.969	2.964	0.000	0.000	0.000	−4.05	−16.53
30	20	216.90	216.90	211.04	7.31	38.76	3.457	2.921	3.288	3.028		0.000	0.000	0.000	−2.48	−18.53
32	22	218.19	218.19		1.29	40.78	3.628	2.947	3.430	3.054		0.000	0.000	0.000	−0.93	−19.89
[illegible]	[illegible]	[illegible]	[illegible]		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]		[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

Atomic Data and Nuclear Data Tables 144 (2022) 101488

First part: even-even nuclei

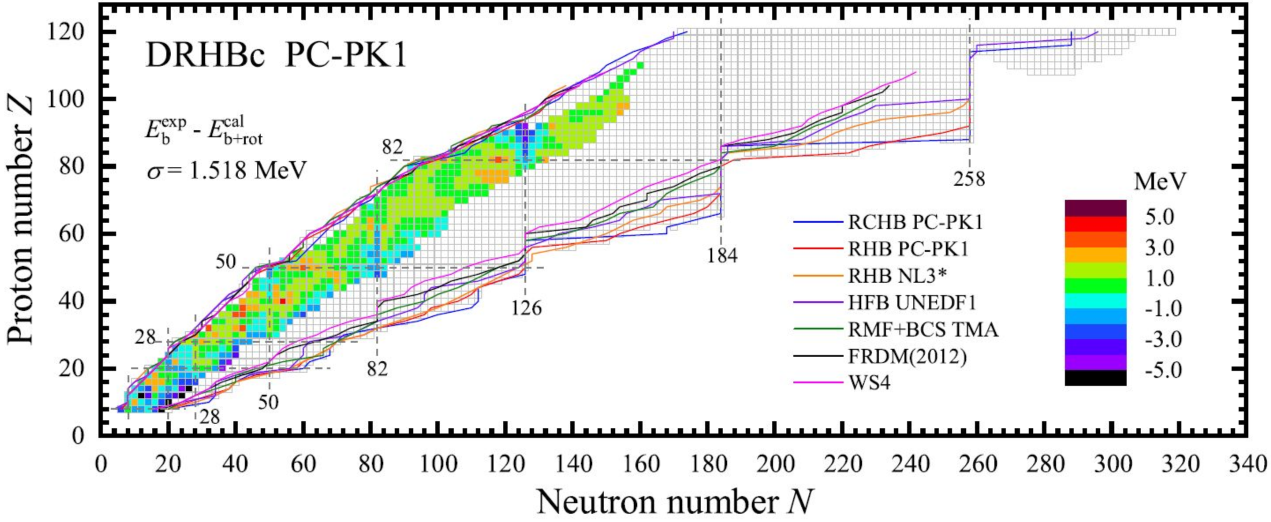


The rms deviations of binding energies, of two-neutron separation energies, and of two-proton separation energies for the DRHBc calculations with PC-PK1 with respect to the AME2020 data [14] in the unit of MeV. The results of other relativistic and non-relativistic density functional calculations are also listed for comparison.

Model	Symmetry	Density functional	$\sigma(E_b)$	$\sigma(S_{2n})$	$\sigma(S_{2p})$	Data numbers	Reference
DRHBc$^{w/o\ E_{rot}}$	Axial	PC-PK1	**2.744**	**1.067**	**0.959**	637	This work
DRHBc$^{w/\ E_{rot}}$	Axial	PC-PK1	**1.518**	**1.104**	**1.095**	637	This work
RCHB	Spherical	PC-PK1	8.036	1.573	1.587	630	[77]
RHB$^{w/o\ E_{corr}}$	Triaxial	PC-PK1	2.635	1.064	0.929	628	[78]
RHB$^{w/\ E_{corr}}$	Triaxial	PC-PK1	1.335	0.751	0.755	628	[78]
RHB	Axial	DD-ME2	2.377	1.007	0.878	636	[73]

Atomic Data and Nuclear Data Tables 144 (2022) 101488

First part: even-even nuclei



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Atomic Data and Nuclear Data Tables 144 (2022) 10

Next, even-odd nuclei: in progress

arXiv:2205.01329; to appear in Phys. Rev. C

DRHBc Mass Table Collaboration

A broad collaboration among several Chinese and Korean teams

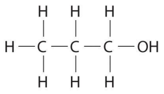
Each team is responsible for calculations within **a given mass region**

- **IBS team: Oxygen-Calcium**

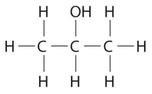
At the same time, **we look for interesting phenomena to study with DRHBc** (e.g., halos, skins, stability peninsulae have been studied)

- **Isomerism and shape coexistence in the O-Ca region**
- **Exotic Shapes: Beads and Dumbells**
- …

Isomerism or shape coexistence



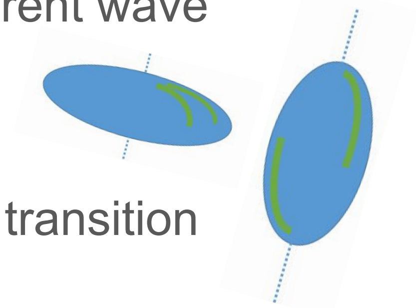
1-Propanol (*n*-propanol)



2-Propanol (isopropanol)

Isomerism in chemistry: Molecules with the same formula (same constituent atoms) but different arrangement of bonds

Isomerism in nuclear physics: Nuclei with same (A,Z) but different wave function, including **different shapes**



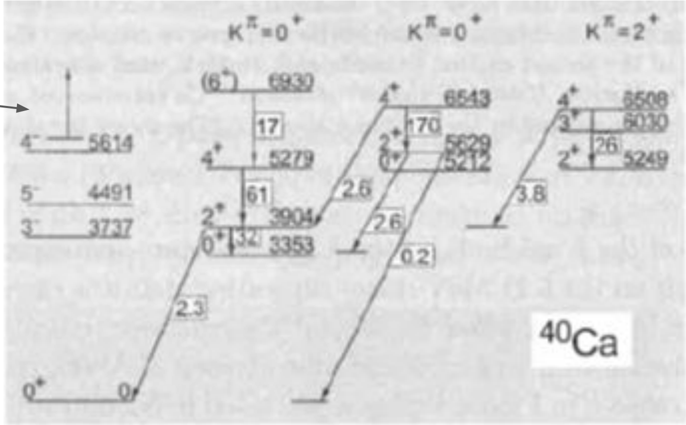
- "Shape coexistence"
- Nuclear isomer: a *metastable* state which is long lived if the transition to the ground state is hindered
- More generally, second 0^+ state close to the ground state
- The energy difference may be quite small
- Important to identify and account for in nucleosynthesis, reactions

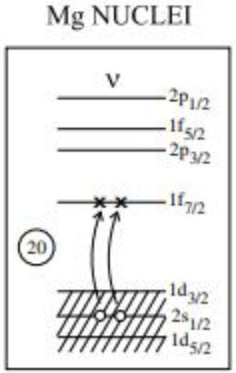
Isomerism or shape coexistence in stable nuclei

Typical signature of shape coexistence: rotational bands with heads other than the ground state

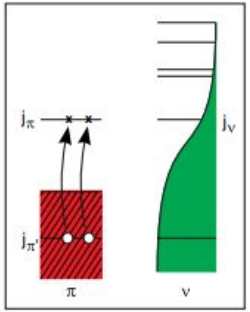
Observed also in magic nuclei

Can be found in many regions of the nuclear chart





Heavy nuclei



K. Heyde, J.L.Wood
Shape coexistence in atomic nuclei
Rev. Mod. Phys. 83, 1476

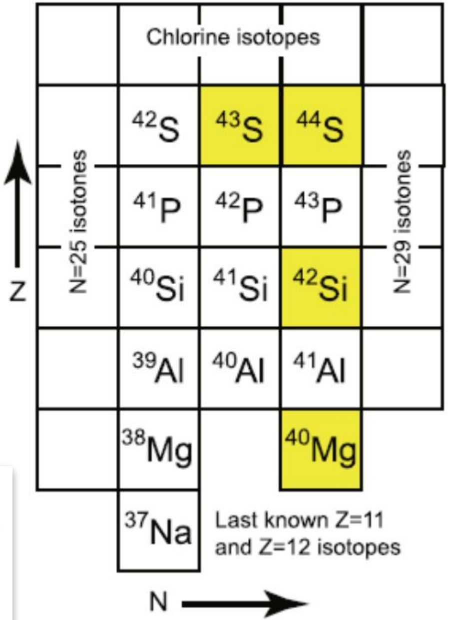
Isomerism or shape coexistence in exotic nuclei

Examples in the O-Ca region of interest:

- S-43 Isomer was discovered at 320 keV (ToF)
- Hindered transition was attributed to the very different wave functions and deformation of the isomer and the g.s.
- S-44 : 0_2^+ state at 1.3MeV

3.1. Shape changes in the sulfur isotopes

Around 2005, the lowest-lying excited 0^+ state of ^{44}S was first identified at GANIL to lie at 1365 keV [32], just 36 keV above the first 2^+ state. The ^{44}S nuclei were produced in the projectile fragmentation of a ^{48}Ca primary beam and implanted into a kapton foil. A fraction of the ^{44}S was produced in the excited 0^+ state which turns out to be long-lived with a half-life exceeding 2 μs [32]. Electron spectroscopy with Si(Li) detectors then allowed to measure the delayed conversion electrons that signal the $0_2^+ \rightarrow 0_1^+$ $E0$ transition. This important



A. Gade, S.N. Liddick
Shape coexistence in neutron-rich nuclei
J. Phys. G 43, 024001

Isomerism or shape coexistence

In DRHBc calculations for Z=8 to 20 we find several cases with two local minima in the potential energy curves, one oblate and one prolate

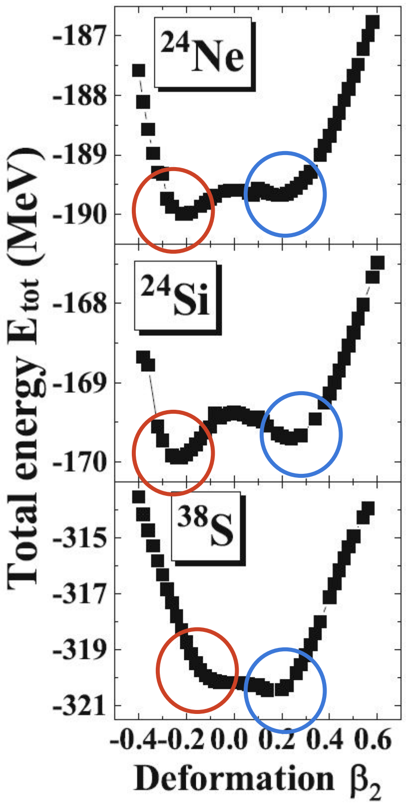
- Shape coexistence?

The two minima typically have very different wave functions, so transitions between them could be hindered

- Isomerism?

The two states can be very close in energy (<1MeV)

Potential energy curves:



[In et al., JKPS77(2020)966]

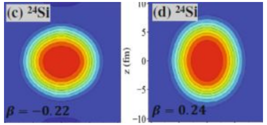
Isomerism or shape coexistence

We surveyed our results (Z=8 to 20) for shape coexistence candidates

Criteria: Two solutions (local minima in PECs) with energy difference < 330 MeV

Findings:

[In et al., JKPS77(2020)966]



- In some cases, one of the solutions is almost spherical
- In some cases, the energy difference is consistent with zero

Isotopes	β_2	ΔE	Isotopes	β_2	ΔE
^{24}Ne	−0.2, 0.18	0.31 MeV	^{32}Ne	−0.04, 0.22	0.02 MeV
^{28}Mg	−0.06, 0.32	0.28 MeV	^{30}Mg	−0.12, 0.24	0.04 MeV
^{24}Si	−0.22, 0.24	0.24 MeV	^{32}Si	−0.18, 0.02	0.30 MeV
^{38}Si	−0.22, 0.24	0.14 MeV	^{28}S	−0.06, 0.32	0.28 MeV
^{38}S	−0.02, 0.14	0.26 MeV	^{46}S	−0.24, 0.26	0.27 MeV
^{48}S	−0.26, 0.18	0.01 MeV	^{50}S	−0.02, 0.02	0.003 MeV
^{52}S	−0.08, 0.08	0.002 MeV	^{32}Ar	−0.2, 0.02	0.24 MeV
^{40}Ar	−0.04, 0.04	0.01 MeV	^{42}Ar	−0.14, 0.14	0.19 MeV
^{62}Ar	−0.08, 0.1	0.02 MeV	^{64}Ar	−0.18, 0.18	0.20 MeV

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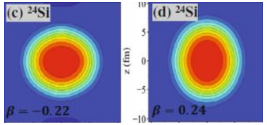

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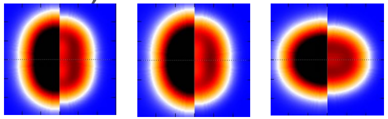
^{62}Ar	−0.08, 0.1	0.02 MeV	^{64}Ar	−0.18, 0.18	0.20 MeV

Generally, detailed spectroscopy in this mass region is advocated

Isomerism or shape coexistence

Shape isomerism with very small energy differences

- Coexistence in production environments (RIBs, astrophysical sites)
- Signatures in gamma transitions?
- ¿ ^{46}S (prolate g.s.) + 2n ↔ ^{48}S* (prolate) ↔ ^{48}S (oblate g.s.) ?
- Depends on timescales of neutron emission and of gamma transitions.



Relation to **transitional nuclei**: shapes between spherical and strongly deformed

[A.Faessler, Rep.Prog.Phys.45, 653]

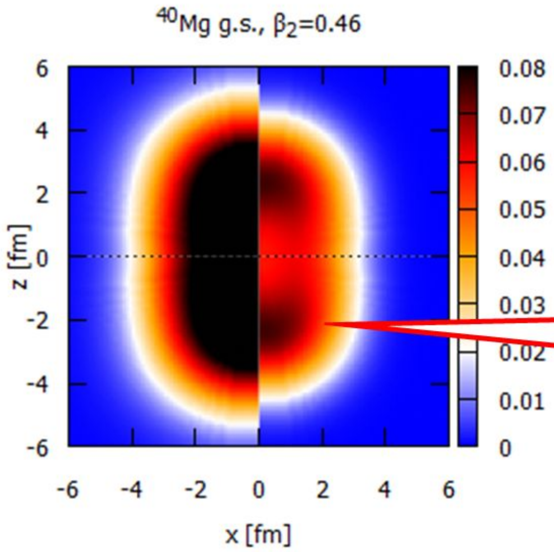
- When angular momentum increases, nuclei can change shape owing to competition of coupling to the core and centrifugal forces; when the shapes are almost degenerate, the transition can take place at low angular momenta

Exotic shapes

Proton and neutron density distributions in the intrinsic frame

Example: Highly deformed Mg-40

- Left half: neutrons
- Right half: protons
- Units: fm^{-3}



Dumbbell shape?

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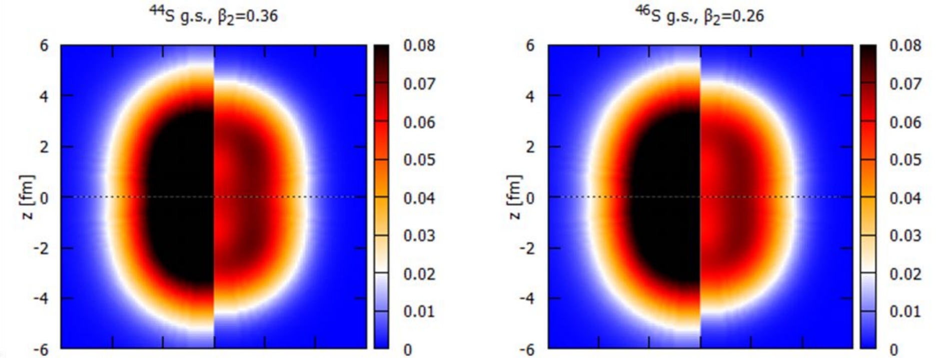
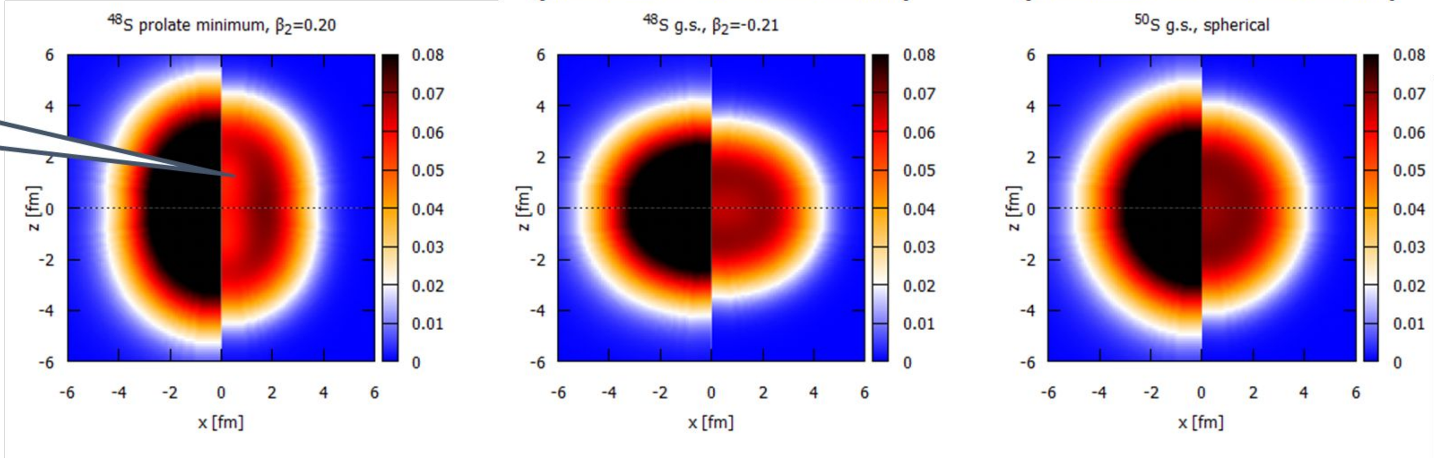
Exotic shapes

Example: S-46 to S-50

- Left half: neutrons
- Right half: protons
- Units: fm^{-3}



Beads?



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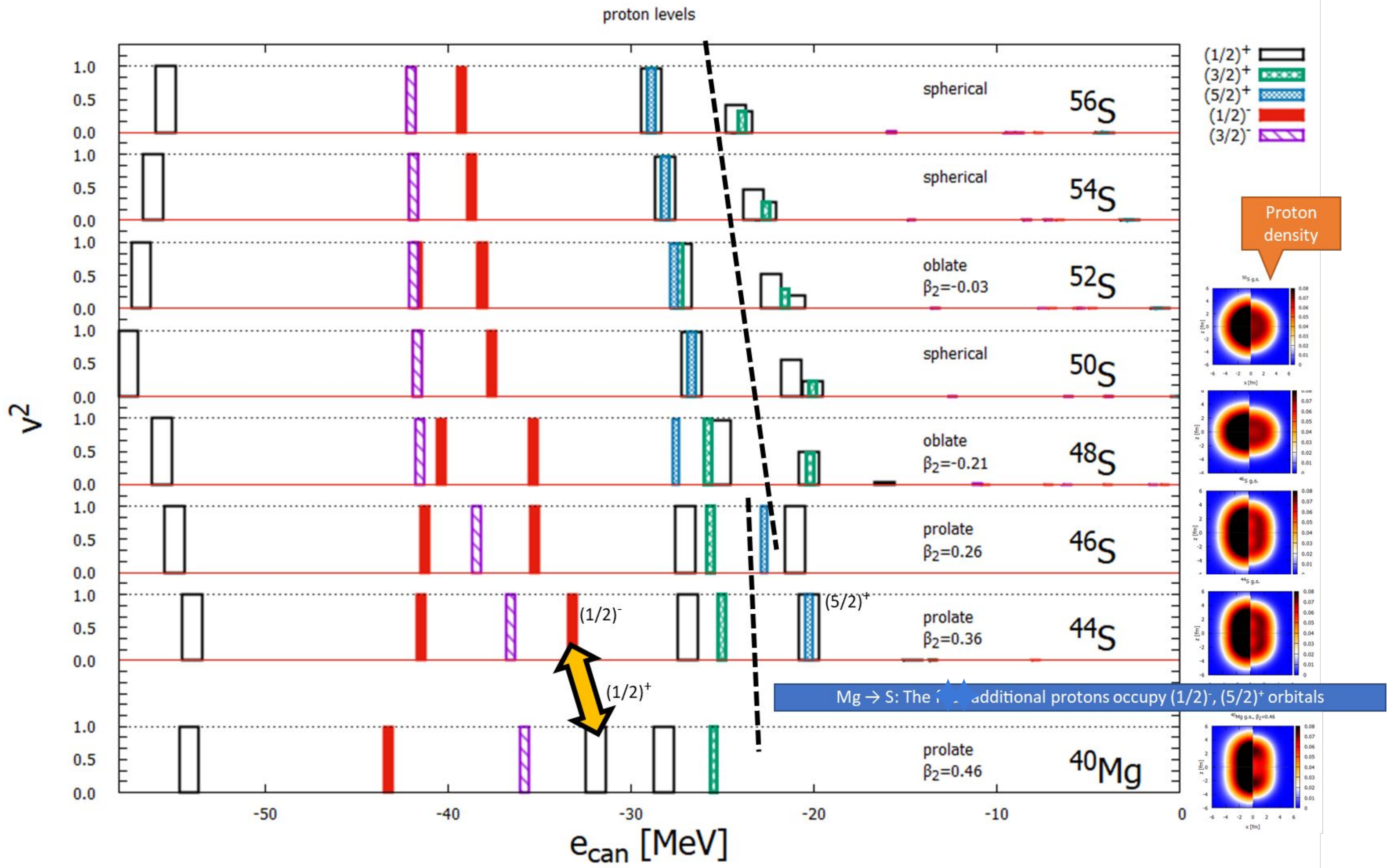
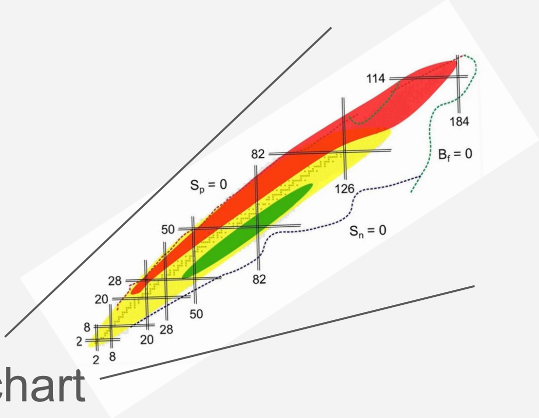


proton levels
v^2
e_{can} [MeV]
$(1/2)^+$
$(3/2)^+$
$(5/2)^+$
$(1/2)^-$
$(3/2)^-$
spherical ^{56}S
spherical ^{54}S
oblate β_2=-0.03 ^{52}S
spherical ^{50}S
oblate β_2=-0.21 ^{48}S
prolate β_2=0.26 ^{46}S
prolate β_2=0.36 ^{44}S
prolate β_2=0.46 ^{40}Mg
$(1/2)^-$
$(5/2)^+$
$(1/2)^+$
Proton density
Mg → S: The additional protons occupy $(1/2)^-$, $(5/2)^+$ orbitals

Summary



Density functional theory

- Nuclear structure and response throughout the nuclear chart
- Our contributions to the study of exotic phenomena in nuclei: *KIDS*, **DRHBc**

DRHBc Mass Table Collaboration

- Building a competitive mass table
- Candidates for shape coexistence and exotic shapes in the light-mass region
- Detailed spectroscopy of neutron-rich nuclei?

감사합니다~~

Thank you!

Related: survival of N=20,N=28 shells

istence in nuclei. If changes in structure as a function of mass number are too sudden, this makes the experimental task of spectroscopic characterization demanding. The only solution to this challenge is to conduct detailed spectroscopy: An excellent example of this is the work of Bednarczyk *et al.* (1998) in the $1f_{7/2}$ shell; cf. Fig. 42. Thus, it will be important in the study of shape coexistence at $N \sim 20$, 28 to carry out detailed spectroscopy of nuclei such as ^{33,34,35}Si, ^{35,36,37}S ($N = 19, 20, 21$) and ^{43,44,45}S, ^{45,46,47}Ar ($N = 27, 28, 29$), because further from stability detailed spectroscopy becomes increasingly challenging and ultimately impossible.

In our perusal of the literature for the neutron-rich $N \sim 20$, 28 region we encountered an active research frontier. While it is premature to present hard and fast interpretations of the emerging structure for these regions, we present a digest of the experimental literature to illustrate the techniques being used, organized by technique.