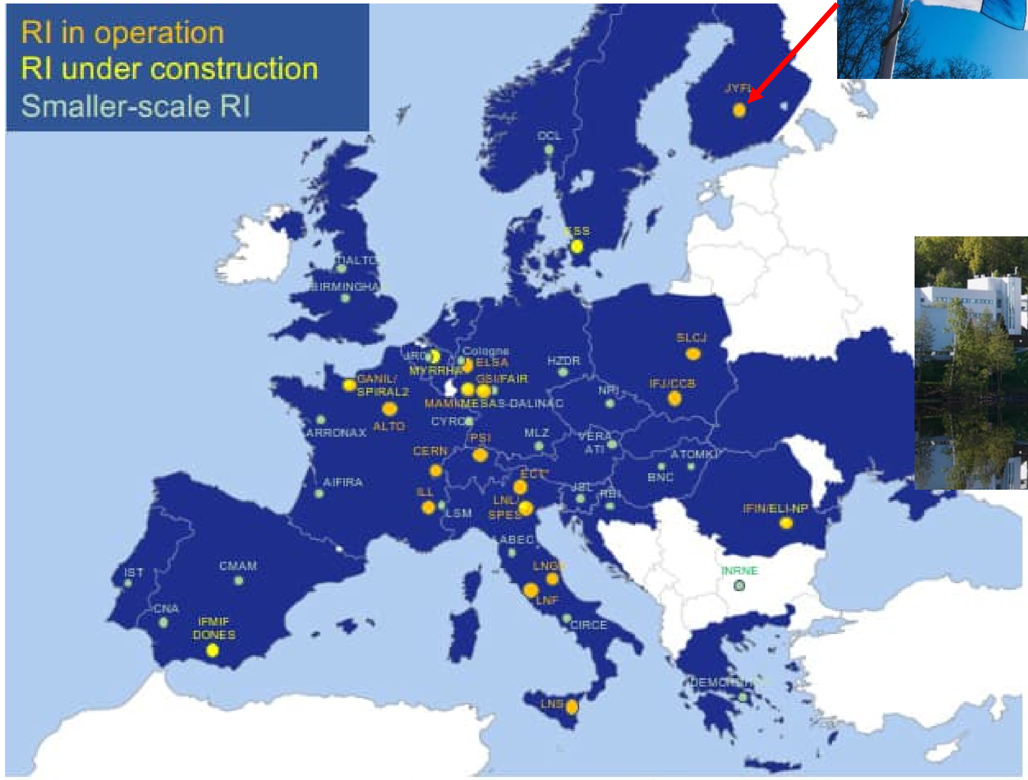
Ground-state properties and techniques

Iain Moore (iain.d.moore@jyu.fi)
Department of Physics,
University of Jyväskylä, Finland

My home base...

UNIVERSITY OF JYVÄSKYLÄ



European landscape of nuclear physics infrastructures.

From the NuPECC Long Range Plan Draft Executive Summary 2024

The northern most Accelerator Laboratory, some 250 km north of Helsinki.

A few remarks

- As this is a school, my goal is to enlighten those of you not already familiar with ground-state properties of nuclei and to present some of the techniques we use to measure them.

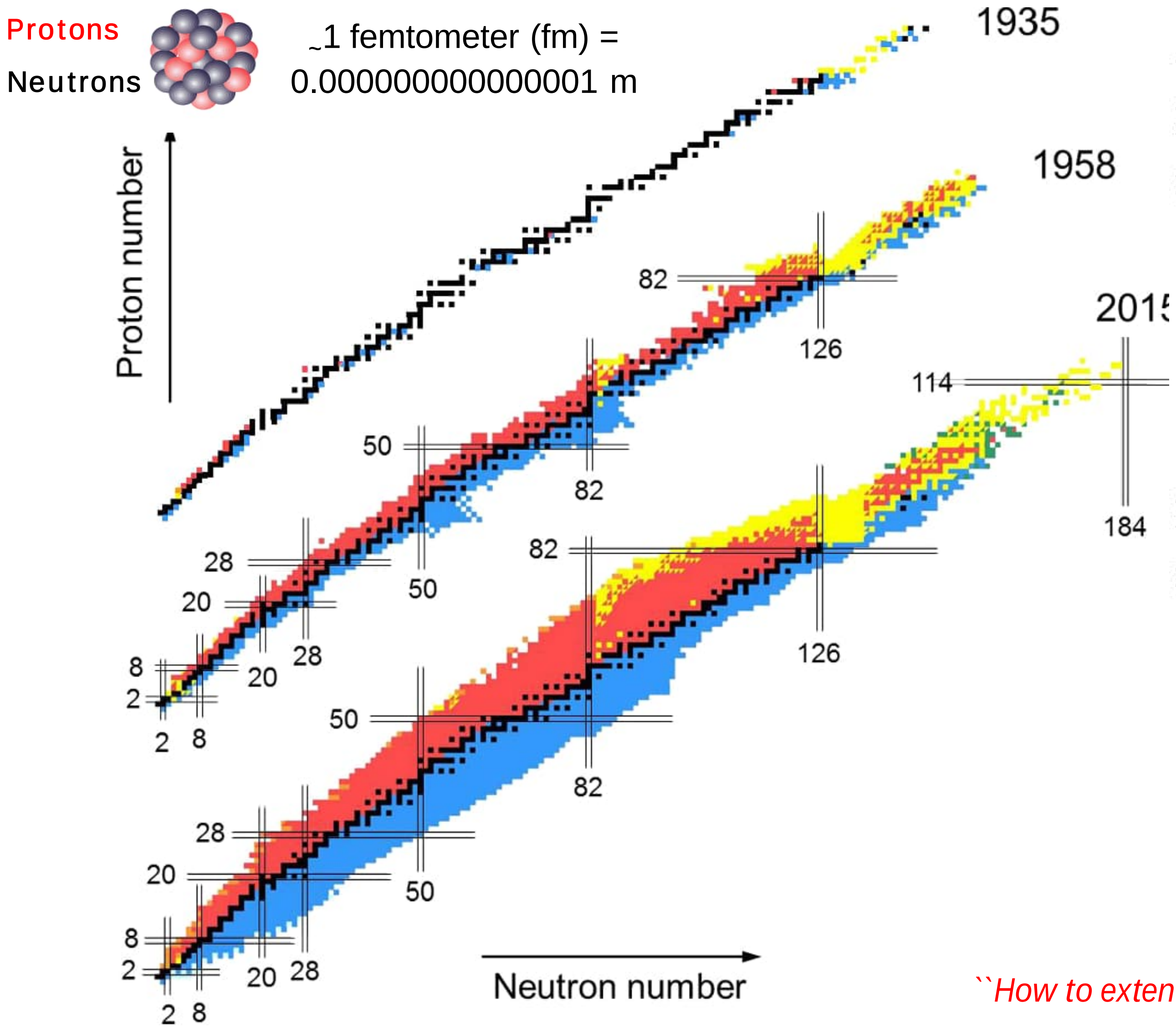
- Interrupt me any time for questions or clarifications. We will also have the Q&A session in the evening.

- Hopefully this will be relaxed...after all, I will sometimes use Comic Sans font in my slides instead of Times New Roman and I swap between black and blue!

- For more single-particle/shell structure, see Sean, for emergent collective structure, Magda. Theory will be tackled by Gianluca.

The chart of nuclides

~1 femtometer (fm) = 0.000000000000001 m



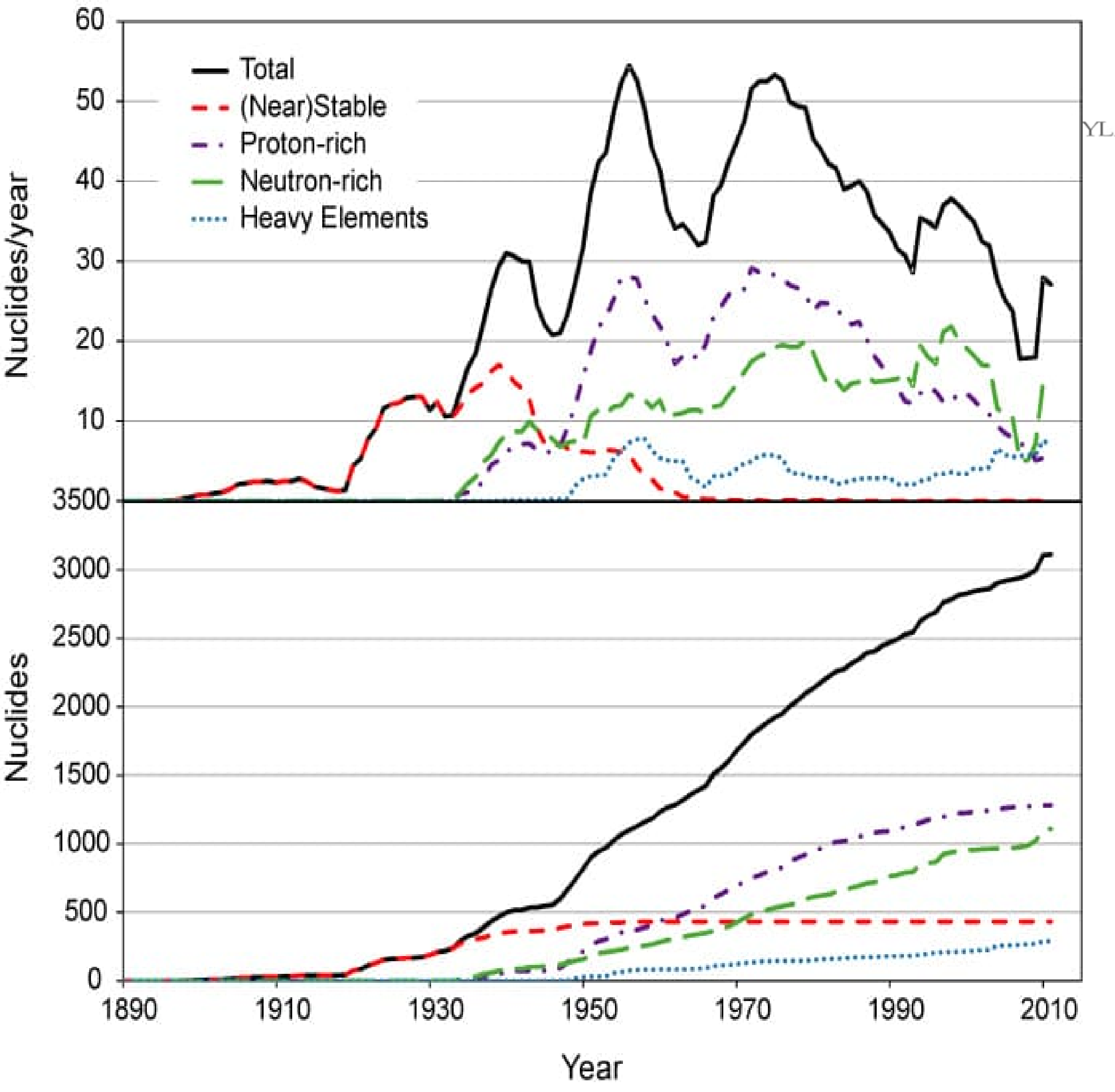
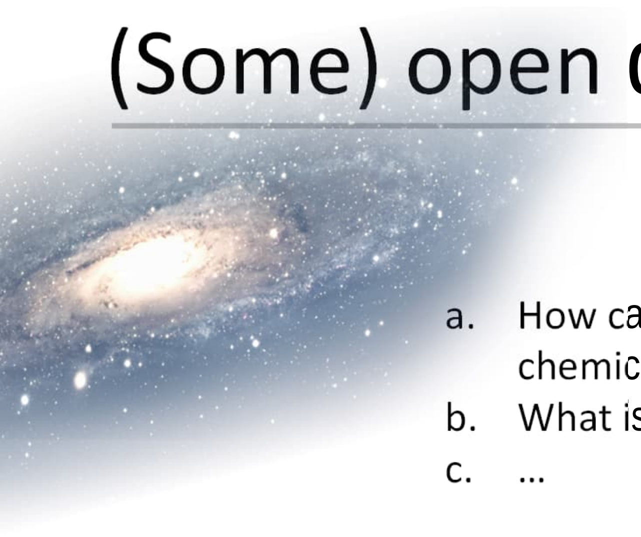


Figure from: M. Thoennessen, Rep. Prog. Phys. 76 (2013) 056301

``How to extend the chart of nuclides?´´, G.G. Adamian et al., EPJ A 56 (2020) 47

(Some) open questions in nuclear physics research

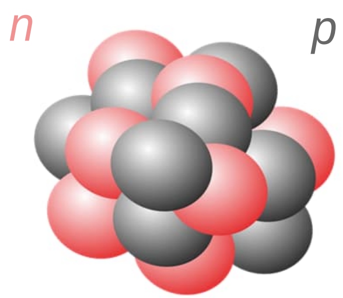


Nuclear Astrophysics

a. How can we better understand the synthesis of heavy elements and the chemical evolution of the visible universe
b. What is the role of the strong interaction in stellar objects?
c. ...

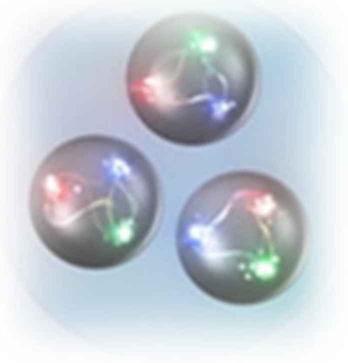
Nuclear structure / nuclear matter

a. What shapes can nuclei take, how do nuclear shells evolve, and what role do nuclear correlations play?
b. What are the limits of the existence of nuclei, and what phenomena arise from open quantum systems?
c. What are the mechanism bind nuclear reactions and nuclear fission?
d. ...



Hadronic physics

a. How does the majority of the visible mass of the universe emergye from the almost massless quarks?
b. What are the properties of the quark-gluon plasma?
c. How do nuclei and nuclear matter emerge from the underlying fundamental interactions?



Properties of a (radioactive) nucleus

Weight

Size

Lifetime/decay

Shape

Electromagnetic property

Is it excited or not?

Outline of my two lectures

Lecture 1: Nuclear ground state properties

- The atomic mass, nuclear binding energy and nuclear structure
- Nuclear fingerprints on atomic lines – the isotope shift
- Hyperfine structure

Lecture 2: Techniques of optical spectroscopy and selected results

- A short introduction to radioactive ion beam production
- Laser resonance ionization
- Doppler-free laser spectroscopy
- What can we learn from charge radii, nuclear moments and spins?

The Atomic Mass in a nutshell

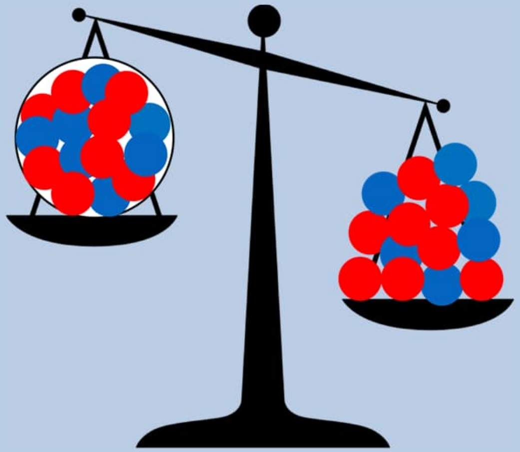
- $m(\mathrm{A,Z}) = Zm_p + (A-Z)m_n + Zm_e - B(\mathrm{A,Z})$
  - A = mass number = neutron number + proton number
  - Z = proton number (element)
  - B the binding energy
    - Nuclear (~MeV/u), Atomic electrons (eV…keV)
    - Compare to absolute nucleon mass ~1 GeV

- Usually, atomic mass tables list the mass defect or excess rather than atomic mass:

$$\boxed{\Delta\left({}^{A}X\right) = \left[m(Z,N) - Au\right]c^2}$$

- ”u” is the atomic mass unit (Definition: m(^{12}C) = 12 u exactly)
- keV/c^2 (1 u = 931494.10242(28) keV/c^2 CODATA2018)

Nuclear Binding Energy



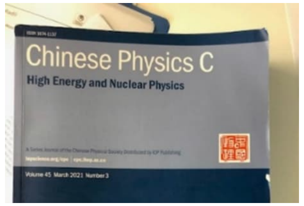
$$M_{atom}(Z,N) = M_{nuc}(Z,N) + Zm_e - B_{\mathrm{e}}(Z)$$

$$M_{nuc}(Z,N) = Zm_p + Nm_n + \frac{E(Z,N)}{c^2}$$

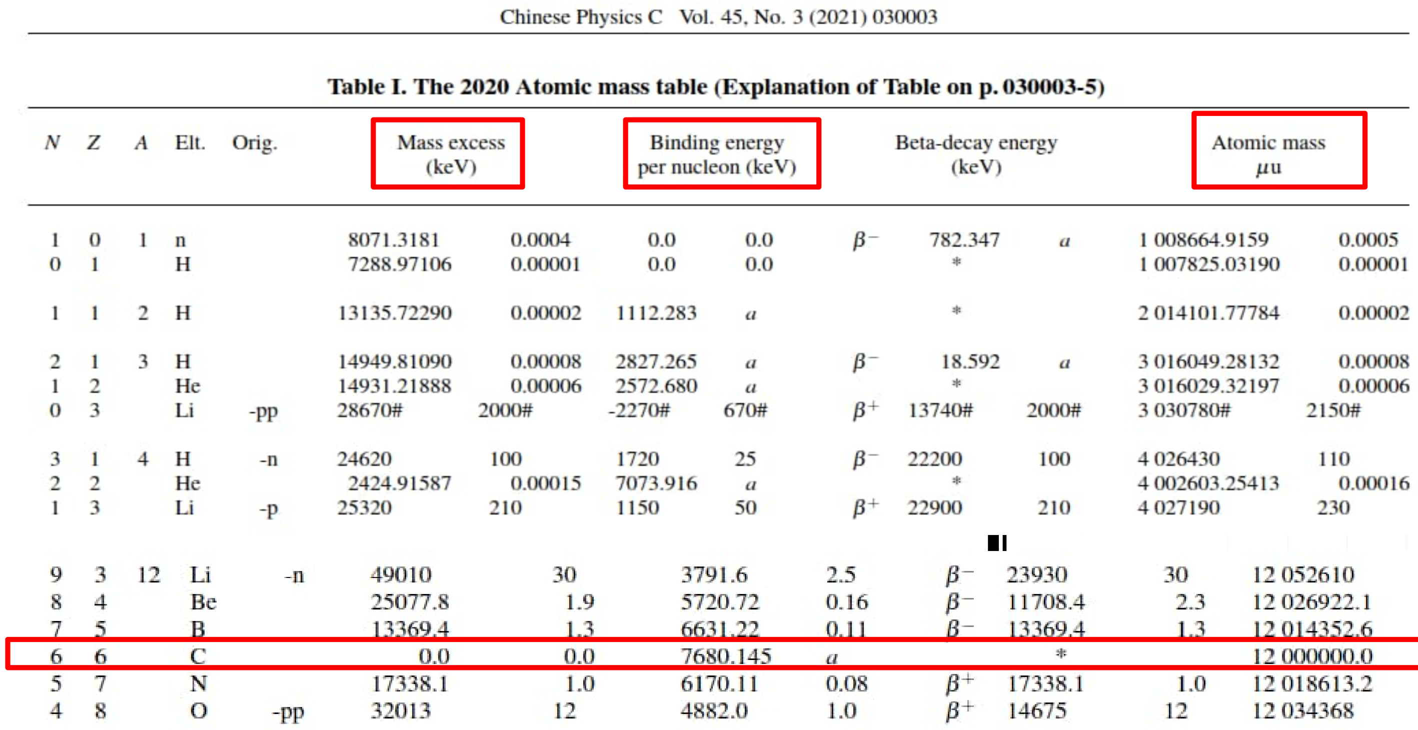
$$\mathrm{E} = mc^2$$

The King James bible for masses: Atomic Mass Table

Periodically published collection of atomic masses



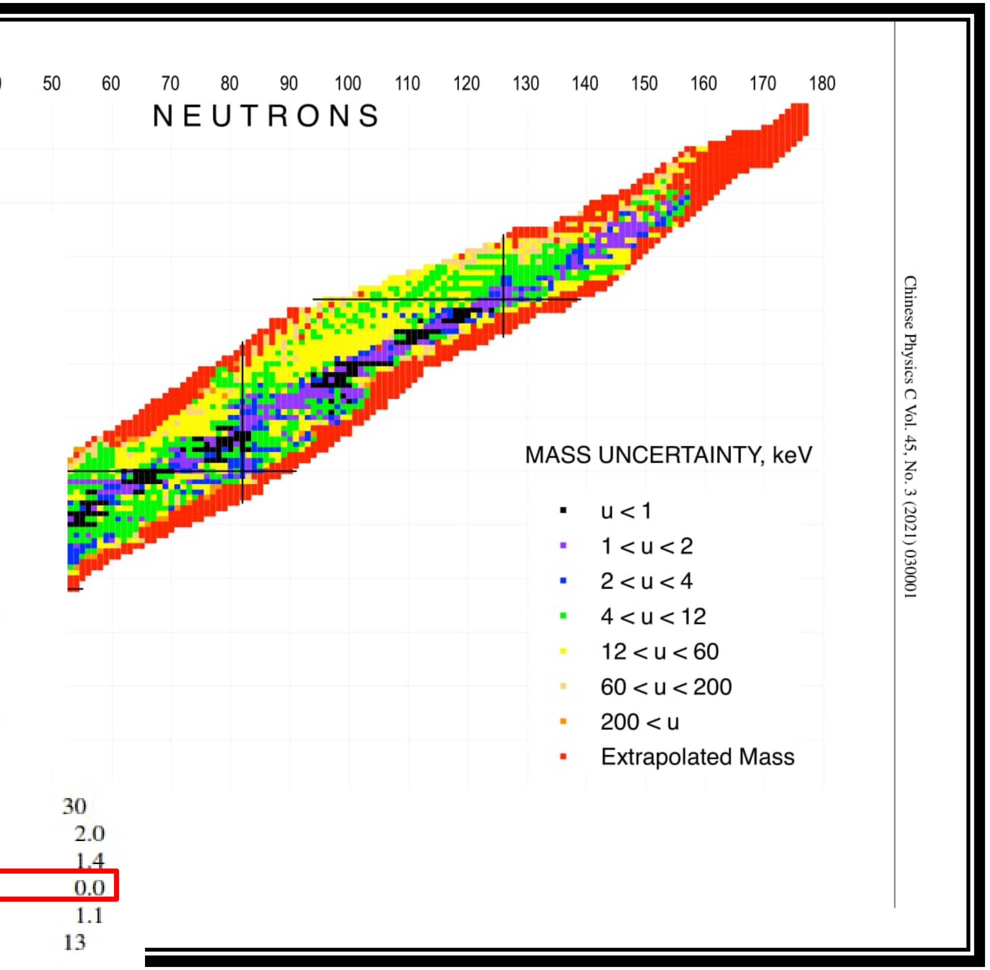
W.J. Huang et al.,
Chinese Phys. C 45,
030002 (2021)



Chinese Physics C Vol. 45, No. 3 (2021) 030003

Table I. The 2020 Atomic mass table (Explanation of Table on p. 030003-5)

N	Z	A	Elt.	Orig.	Mass excess (keV)		Binding energy per nucleon (keV)		Beta-decay energy (keV)			Atomic mass μu	
1	0	1	n		8071.3181	0.0004	0.0	0.0	β^-	782.347	*a*	1 008664.9159	0.0005
0	1		H		7288.97106	0.00001	0.0	0.0		*		1 007825.03190	0.00001
1	1	2	H		13135.72290	0.00002	1112.283	*a*		*		2 014101.77784	0.00002
2	1	3	H		14949.81090	0.00008	2827.265	*a*	β^-	18.592	*a*	3 016049.28132	0.00008
1	2		He		14931.21888	0.00006	2572.680	*a*		*		3 016029.32197	0.00006
0	3		Li	-pp	28670#	2000#	-2270#	670#	β^+	13740#	2000#	3 030780#	2150#
3	1	4	H	-n	24620	100	1720	25	β^-	22200	100	4 026430	110
2	2		He		2424.91587	0.00015	7073.916	*a*		*		4 002603.25413	0.00016
1	3		Li	-p	25320	210	1150	50	β^+	22900	210	4 027190	230
9	3	12	Li	-n	49010	30	3791.6	2.5	β^-	23930	30	12 052610	30
8	4		Be		25077.8	1.9	5720.72	0.16	β^-	11708.4	2.3	12 026922.1	2.0
7	5		B		13369.4	1.3	6631.22	0.11	β^-	13369.4	1.3	12 014352.6	1.4
6	6		C		0.0	0.0	7680.145	*a*		*		12 000000.0	0.0
5	7		N		17338.1	1.0	6170.11	0.08	β^+	17338.1	1.0	12 018613.2	1.1
4	8		O	-pp	32013	12	4882.0	1.0	β^+	14675	12	12 034368	13

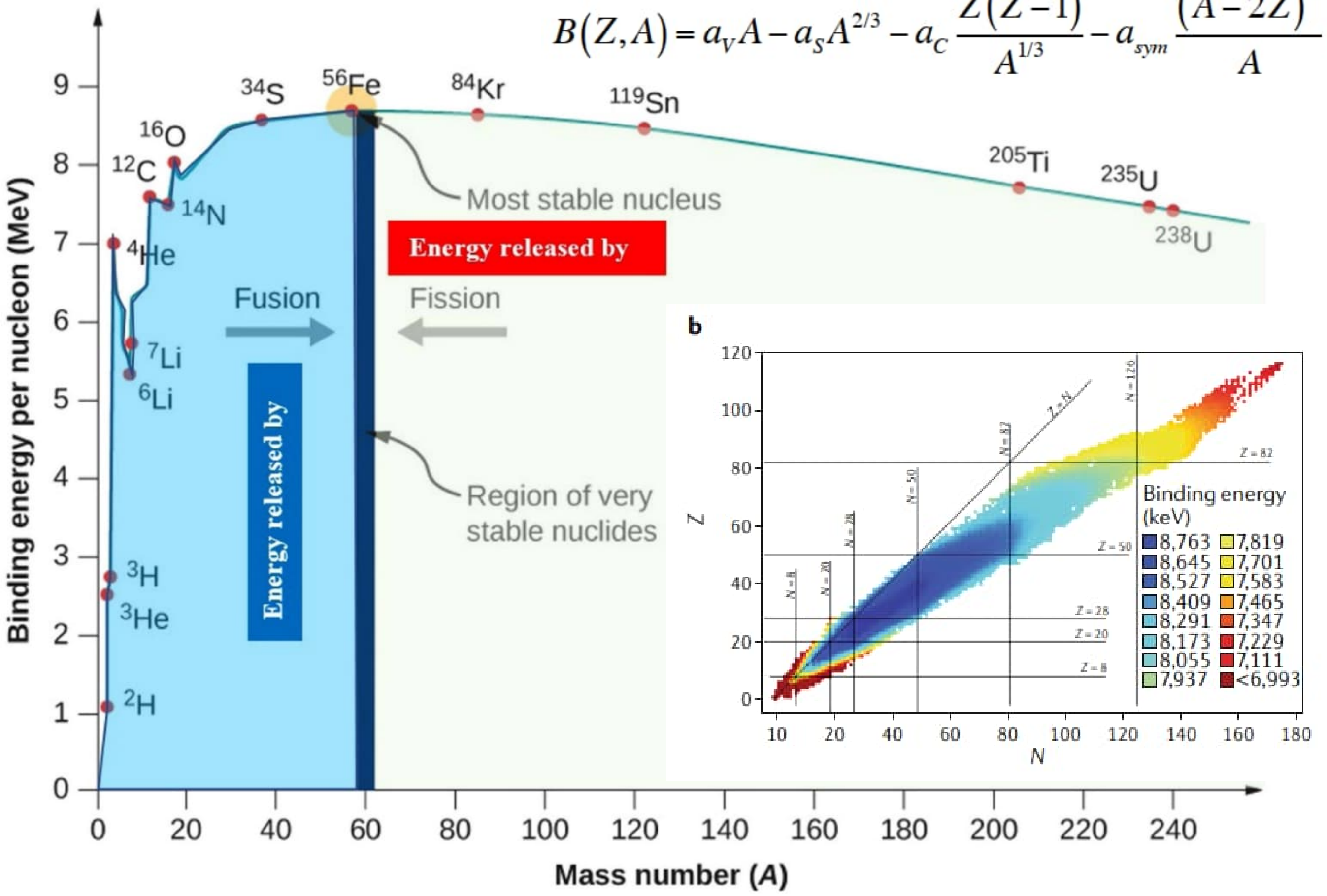


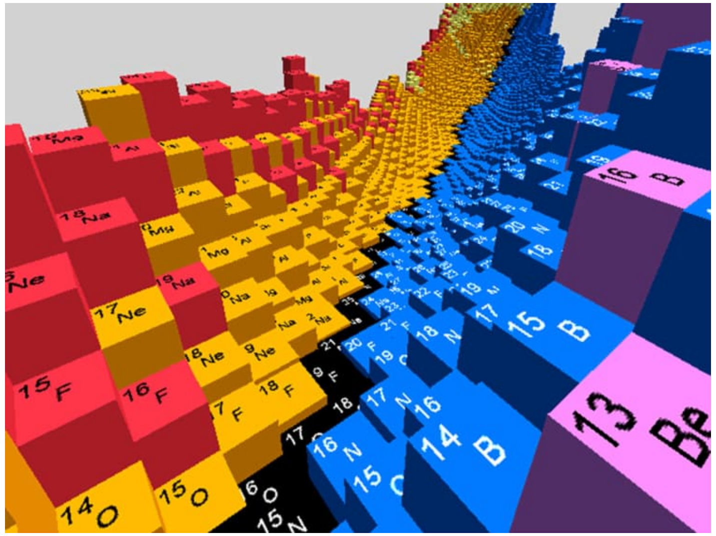
Page 3: Mass-excess uncertainties for all nuclei in ground state

Nuclear binding energy

The energy required to dissasemble a nucleus into its constitents

$$B(Z,A)=a_V A-a_S A^{2/3}-a_C\frac{Z(Z-1)}{A^{1/3}}-a_{sym}\frac{(A-2Z)^2}{A}+\delta$$





- When a nucleus is formed, the binding energy occurs due to a transformation of a mass quantity into energy.
- More bound = more binding energy
- Nuclear stability – the nuclear landscape!
- Theory is needed to predict the limits of stability.
- Nuclear energy

Figures from L.S. Paraschiv et al., Energy Reports 8 (2022) 342; P. Schwerdtfeger et al., The periodic table and the physics that drives it, Nature Reviews Chemistry (2020)

Why to measure atomic masses?

$$\nu_c = \frac{1}{2\pi}\frac{q}{m}B$$

Mass of each and every nuclear state is important!

- Some masses are needed with more precision, some less…

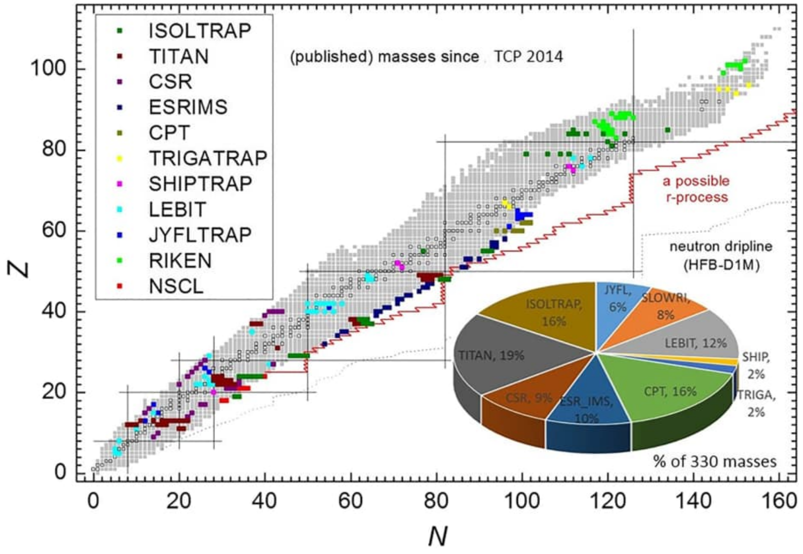


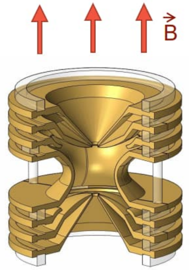
Figure from D. Lunney, Hyp. Int. 240 (2019) 48

~2500 masses experimentally determined (white boxes)

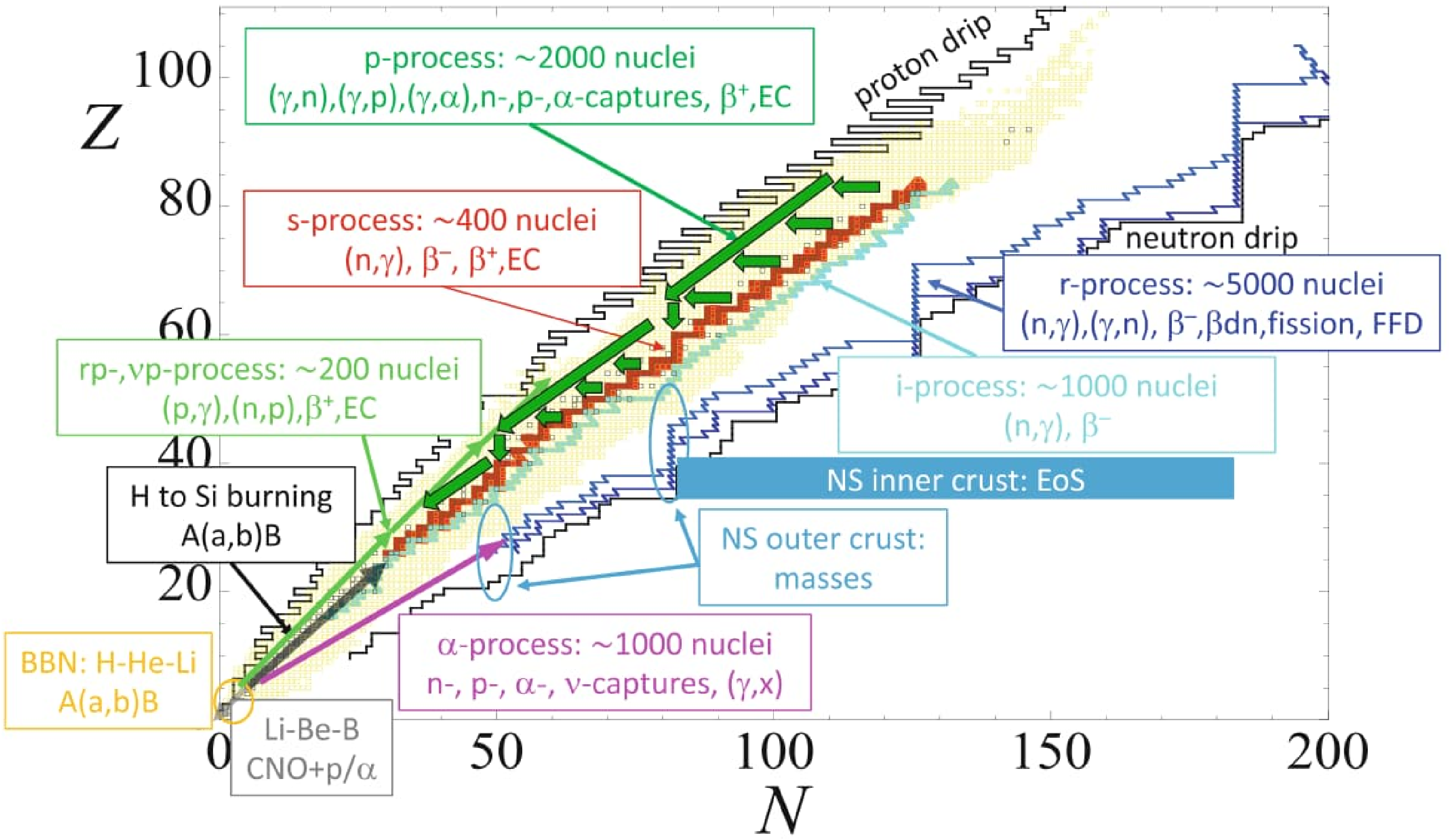
	δm/m	δm for m=100 u (μu)	δm for m=100 u (keV)
General physics & chemistry	≤ 10^{-5}	1000	1000
Nuclear structure physics - separation of isobars	≤ 10^{-6}	100	100
Astrophysics - separation of isomers	≤ 10^{-7}	10	10
Weak interaction studies	≤ 10^{-8}	1	1
Metrology - fundamental constants Neutrino physics	≤ 10^{-9}	0.1	0.1
CPT tests	≤ 10^{-10}	0.01	0.01
QED in highly-charged ions - separation of atomic states	≤ 10^{-11}	0.001	0.001

MR-TOF

Penning traps



Nuclear masses for astrophysics



"Masses of exotic nuclei", from the Handbook of Nuclear Physics (2022)

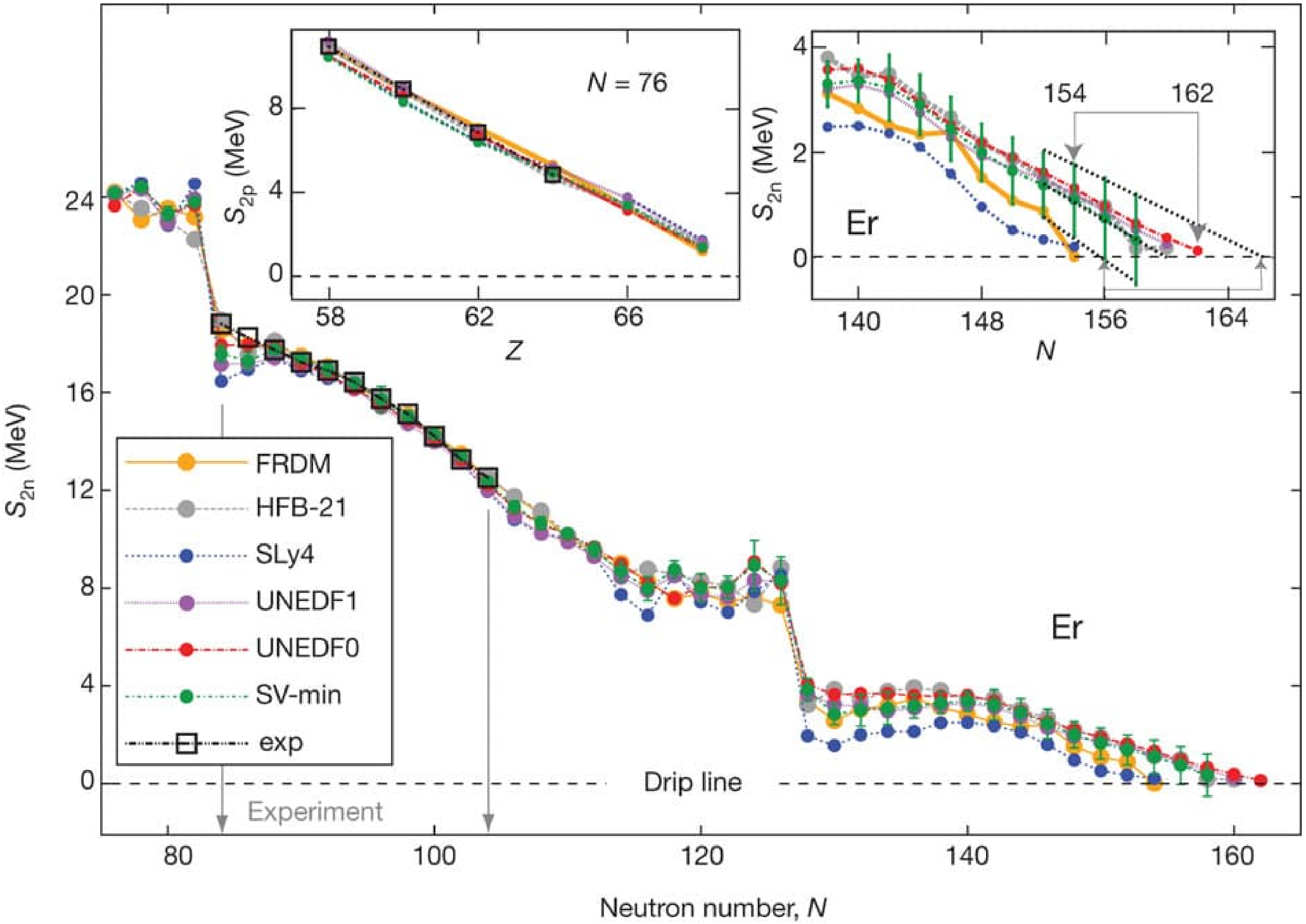
- Nuclear masses (binding energies) determine nucleosynthesis pathways
- Modeling the rp process:

  - X-ray bursts and light curves
  - proton captures have exponential dependence on mass

- Theoretical models are critically important, e.g., for modeling the r-process

See nuclear astrophysics lectures by Ann-Cecilie!

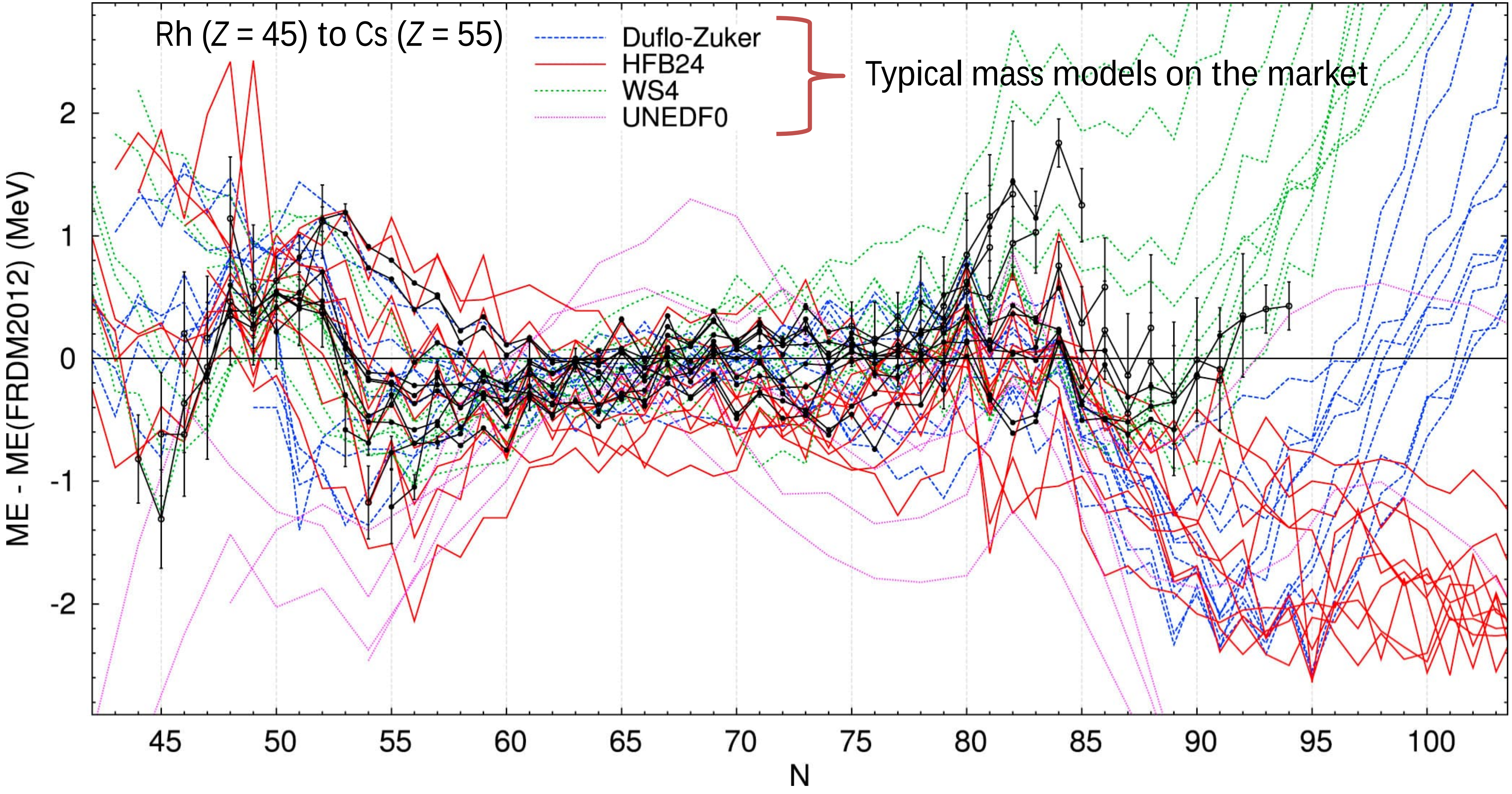
Calculated and experimental S_{2n} for erbium



- Stable Er ($Z = 68$) isotopes from $N = 94$ to $N = 102$.
- S_{2n} = two-neutron separation energy
- $S_{2n} = 0$ is the neutron drip line
- S_{2p} = two-proton separation energy

Figure from J. Erler et al., Nature 486 (2012) 509.

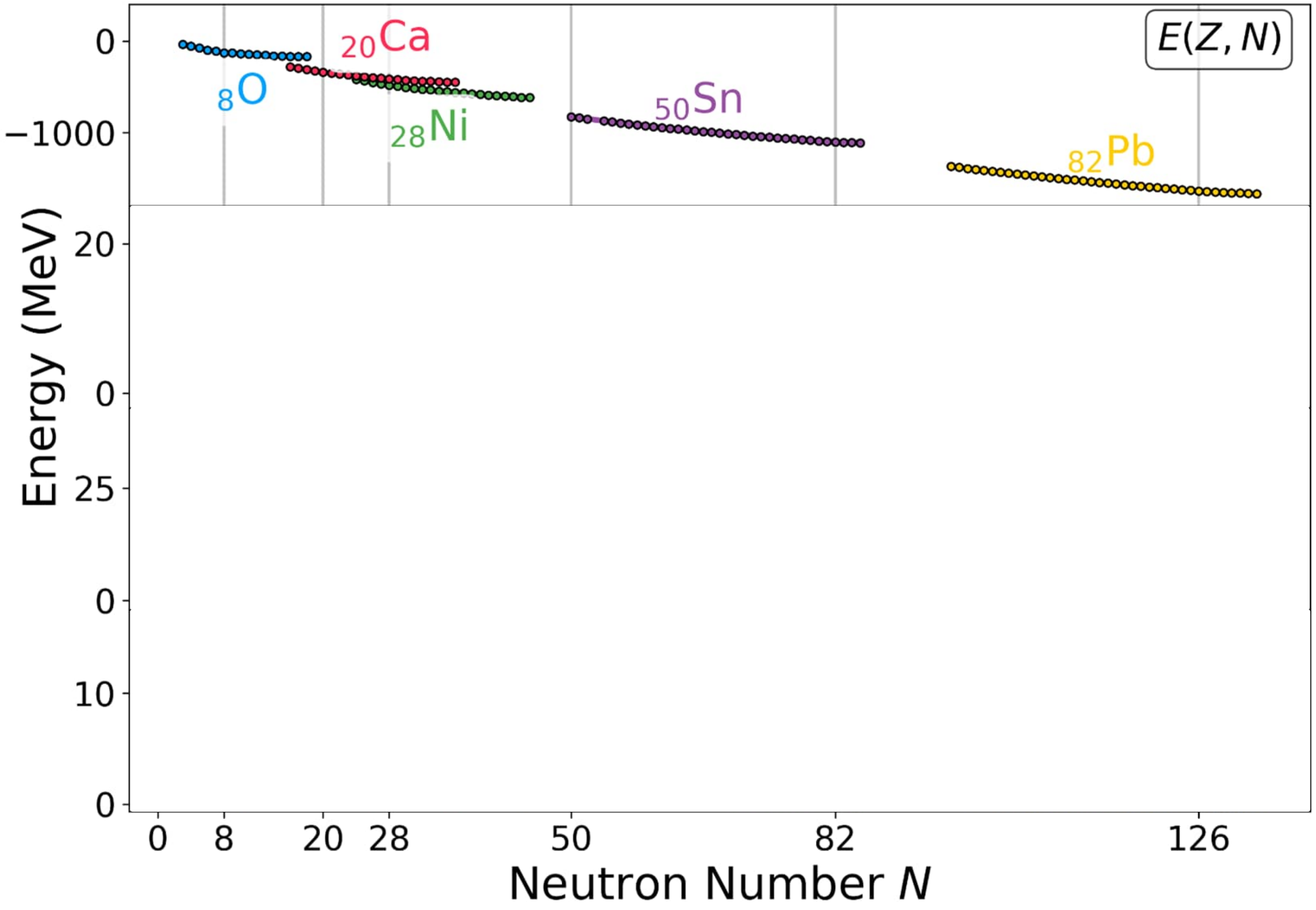
Mass extrapolations towards exotic nuclei



Typical mass models on the market

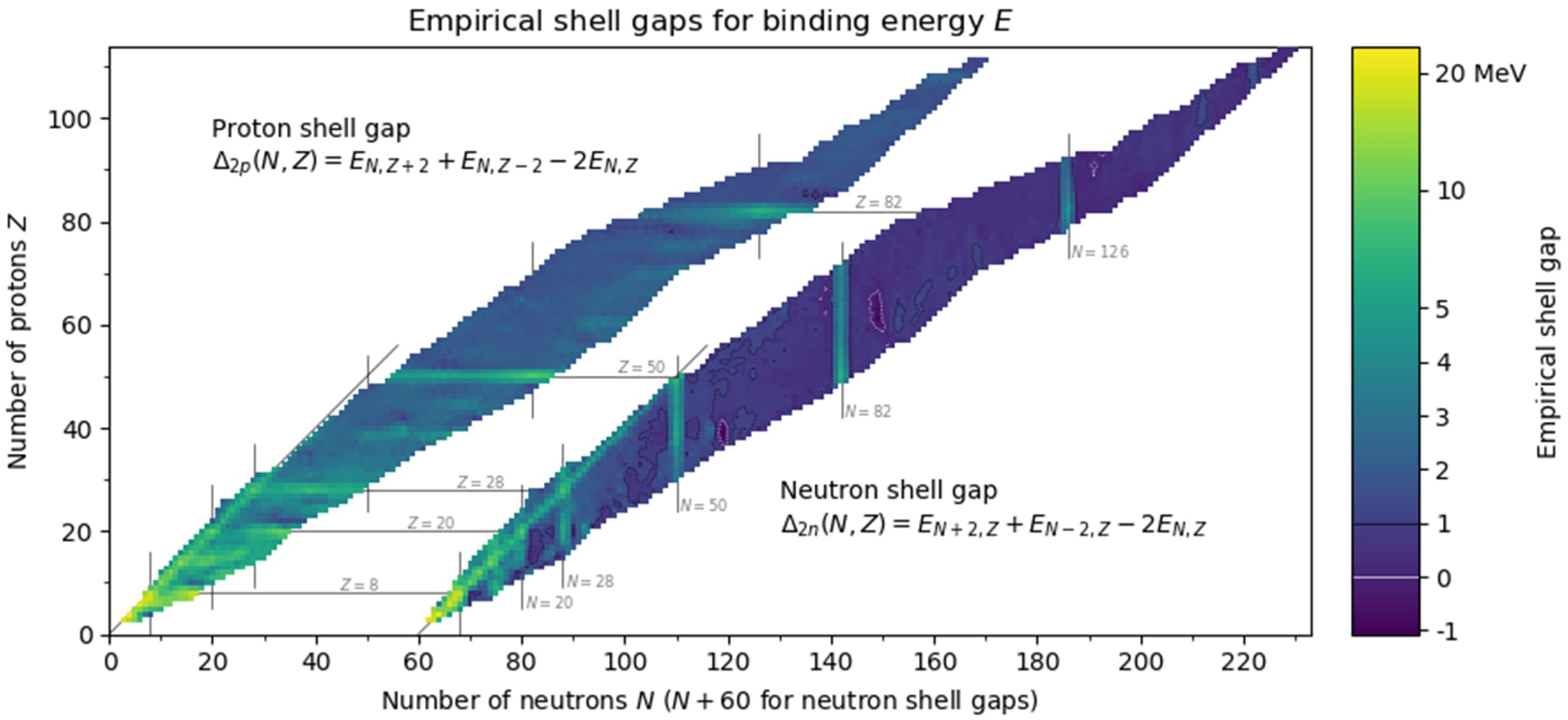
From "Ion traps in nuclear physics – Recent results and achievements", T. Eronen et al., PPNP 91 (2016) 259

Nuclear structure via mass probes



Courtesy of Lukas Nies, PLATAN 2024 conference.

Highlighting the empirical shell gaps



Properties of a (radioactive) nucleus

Weight

Size

Lifetime/decay

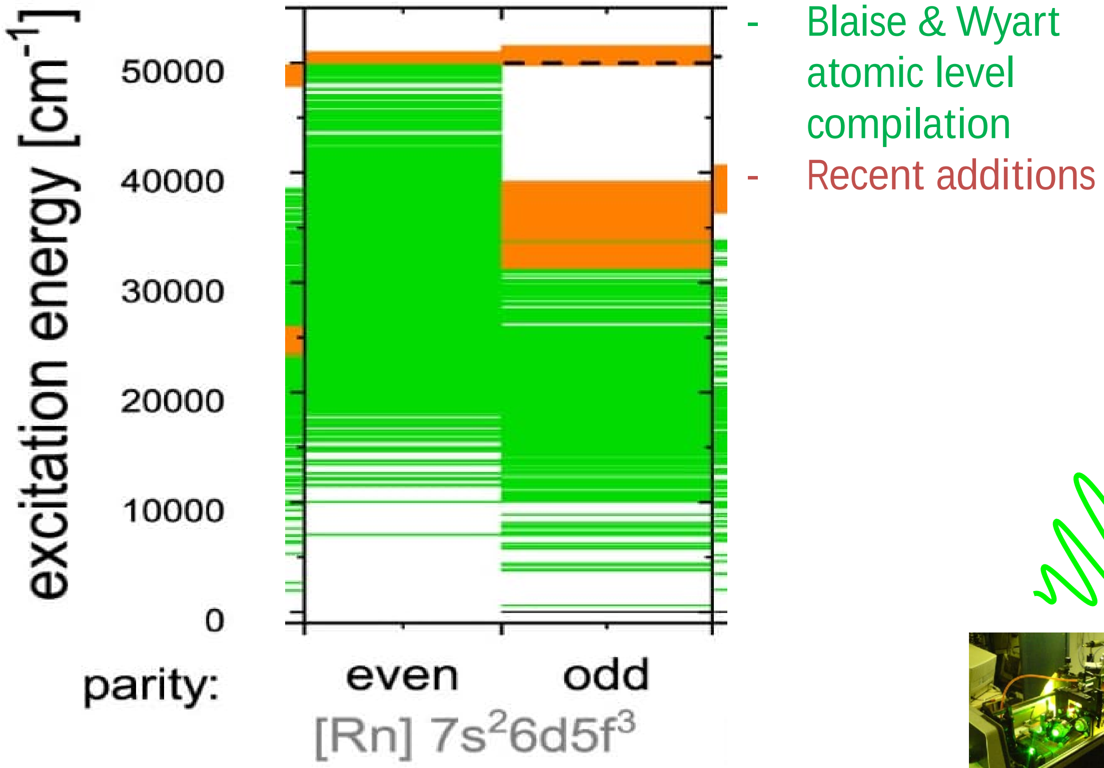
Shape

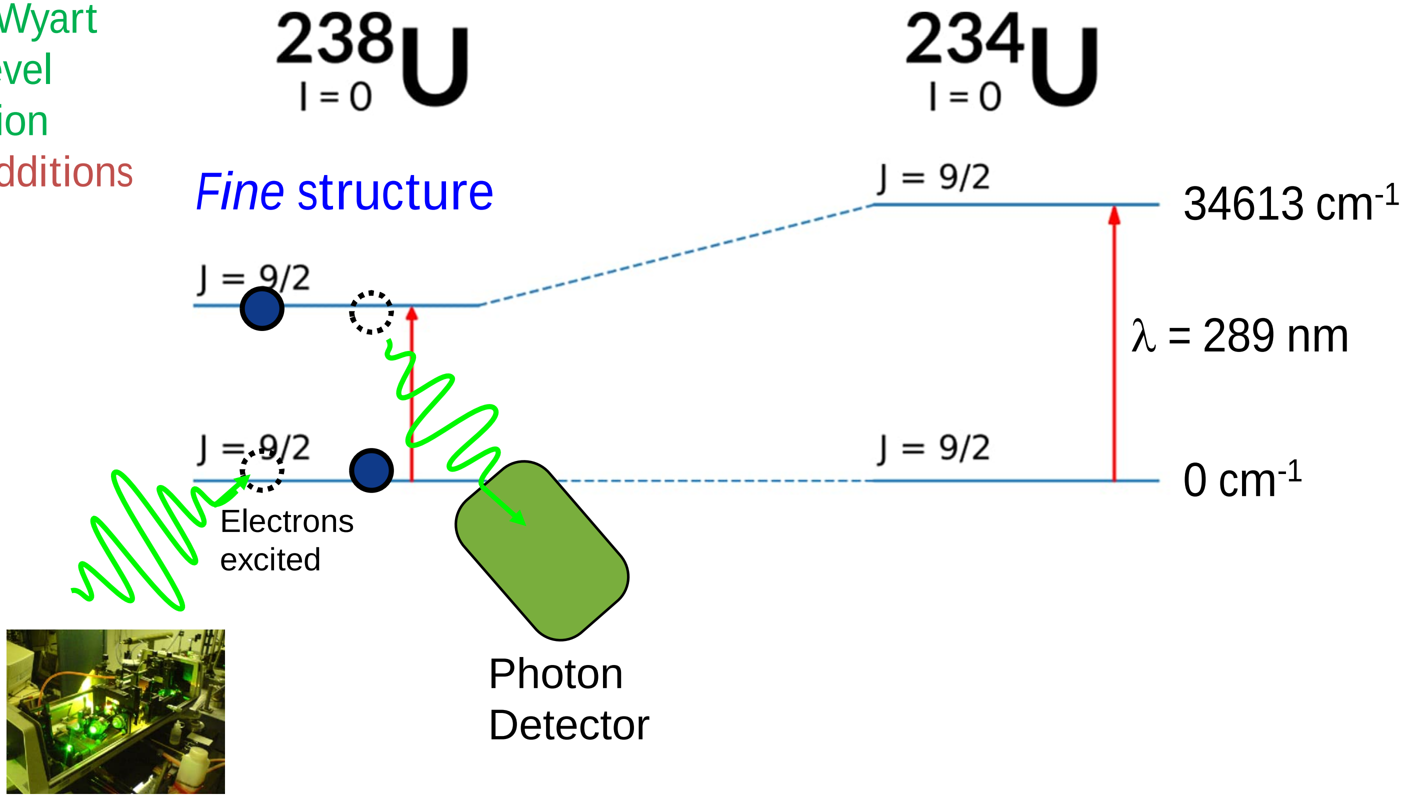
Electromagnetic property

Is it excited or not?

Nuclear properties via the atomic fingerprint

Uranium atom

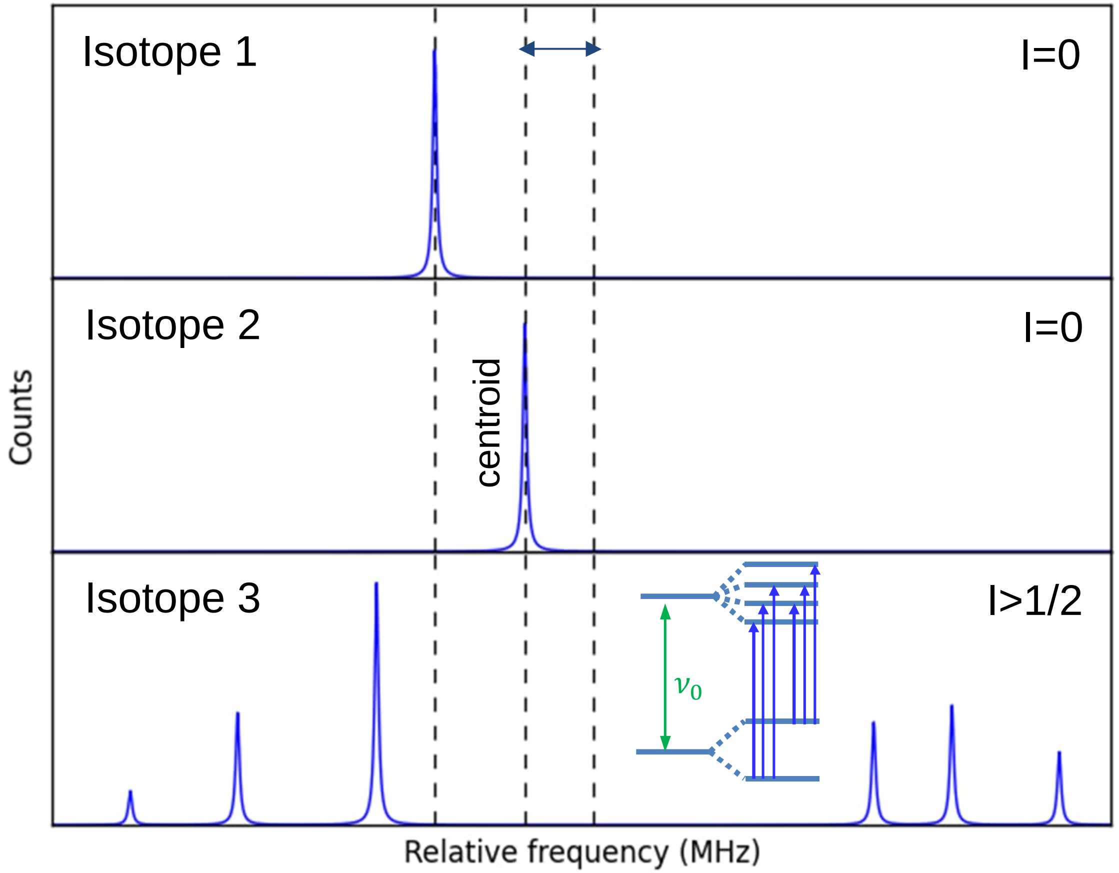




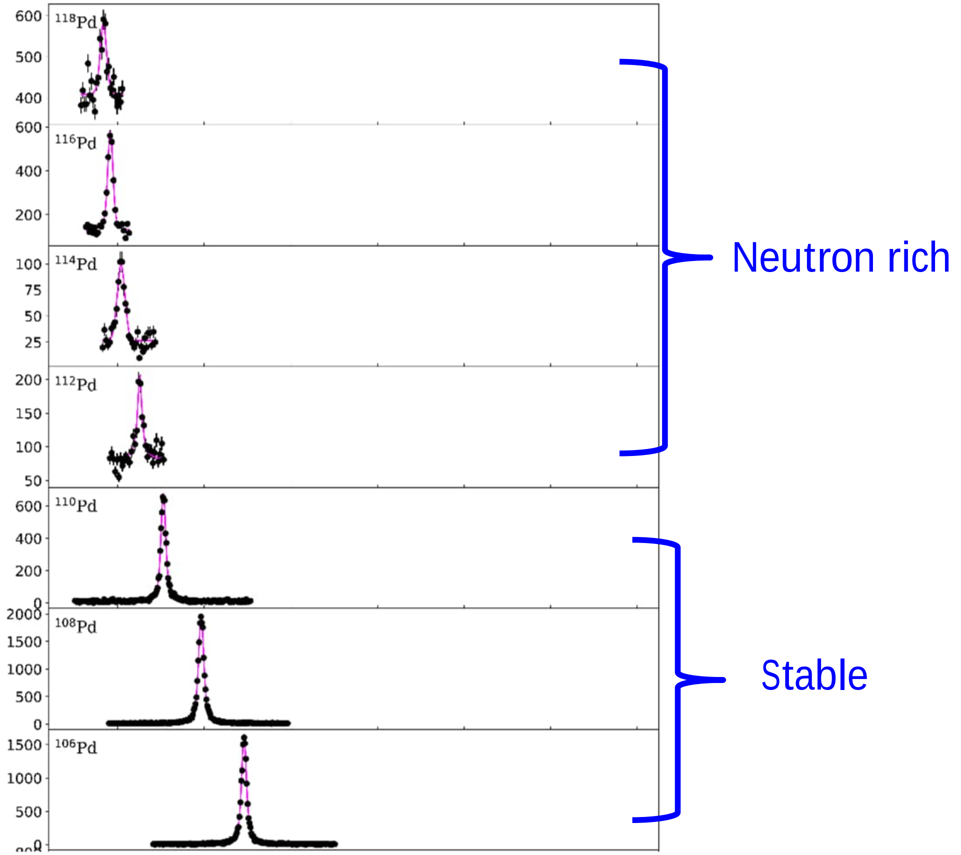
Note: the heaviest of elements, e.g., Lr with Z=103, only theoretical estimates for atomic levels exist!

1 cm^{-1} : ~30000 MHz (30 GHz)
1 eV: ~8000 cm^{-1}

Isotope shifts of electronic transitions



Even mass Pd (Z = 46) isotope shifts



The isotope shift is the frequency difference in an electronic transition between two isotopes of mass A and A´

$$\delta\nu^{AA'} = \nu^{A'} - \nu^{A}$$

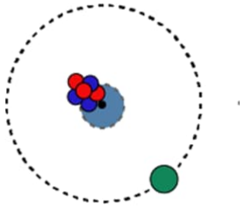
What causes the isotope shift?

The shift in the atomic transition frequency between different isotopes of the same element arises due to changes in nuclear mass and nuclear size.

$$\delta\nu_{IS} = \delta\nu_{MS} + \delta\nu_{FS}$$

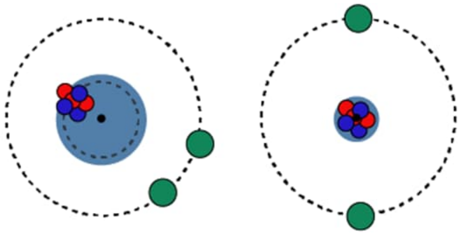
Mass shift

Normal Mass shift



$$= \nu m_e \frac{m_{A'} - m_A}{m_A \, m_{A'}}$$

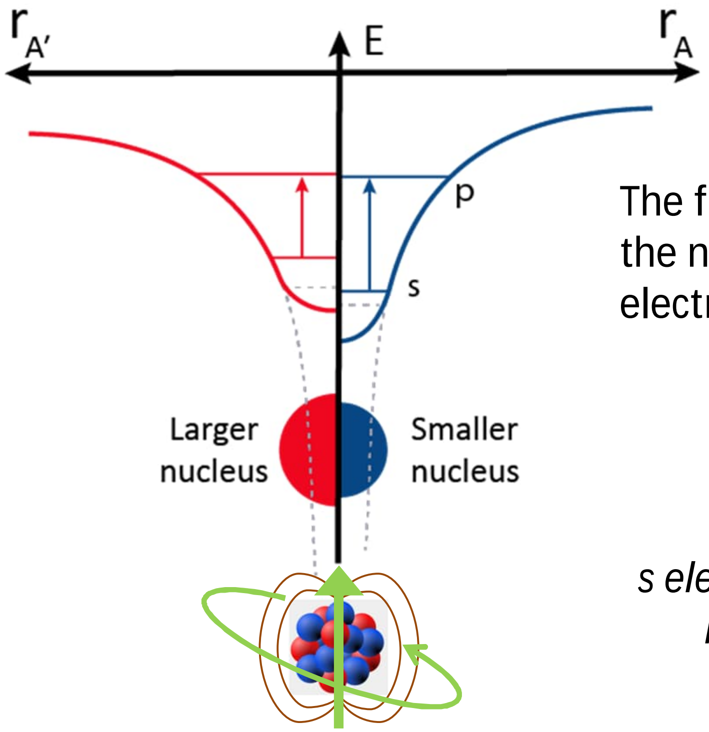
Specific Mass shift



takes into account correlations of the electron motion

Field shift

Nuclear radius: few × 10^{-15} m
Atomic radius: few × 10^{-10} m



The finite spatial extent of the nucleus perturbs the electron wavefunction.

s electrons for example are more tightly bound

From the isotope shift to the nuclear size

R

$$\delta\nu_i^{A,A'} = \nu_i^{A'} - \nu_i^{A} = K_i \overbrace{\frac{m_{A'} - m_A}{m_A\, m_{A'}}}^{\text{Mass shift}} + \overbrace{F_i\, \delta}^{\text{Field shift}}\langle r^2\rangle^{A,A'}$$

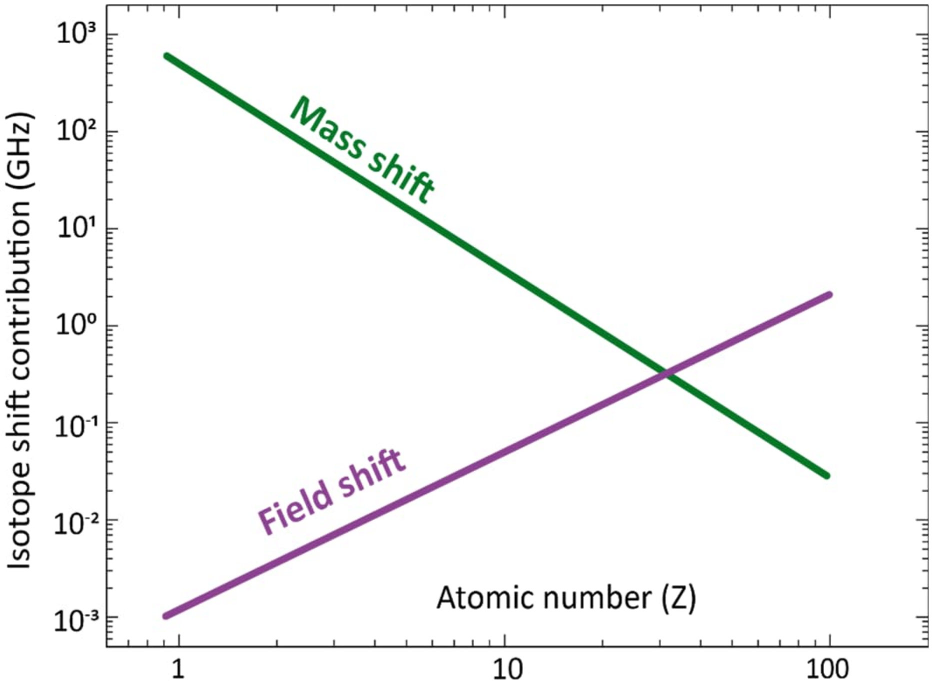
Nuclear mean-square charge radii

EXPERIMENT

THEORY

To evaluate isotope shift data:

- mass data from Atomic Mass Evaluation (2021)
- SMS either calculated (ab-initio, MBPT, coupled cluster...) or evaluated via non-optical data (elastic electron scattering, muonic atom X-rays)
- Field shift factor F from non-optical data, semi-empirical, atomic theory (accurate to ~10%)

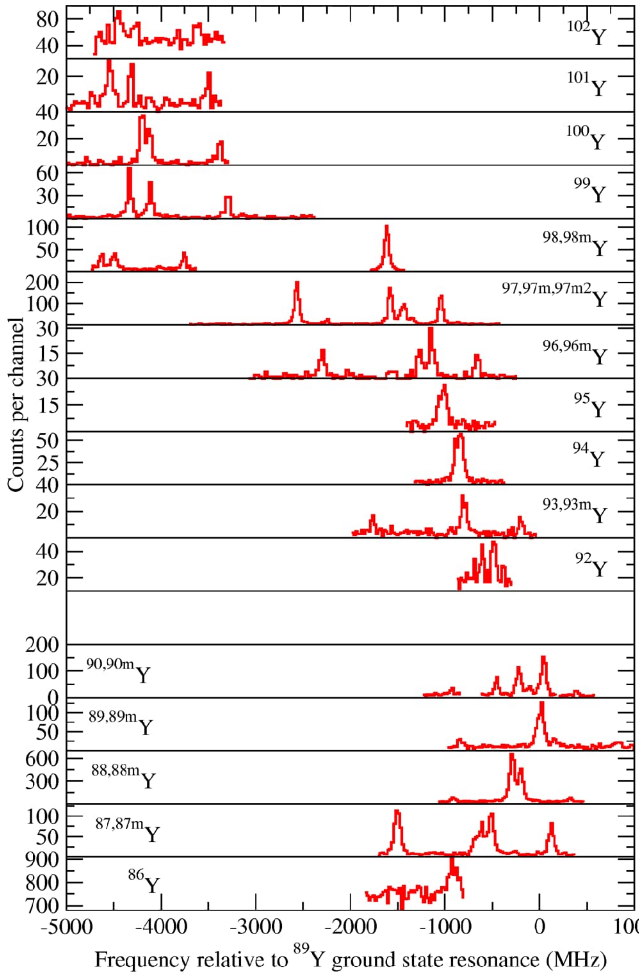


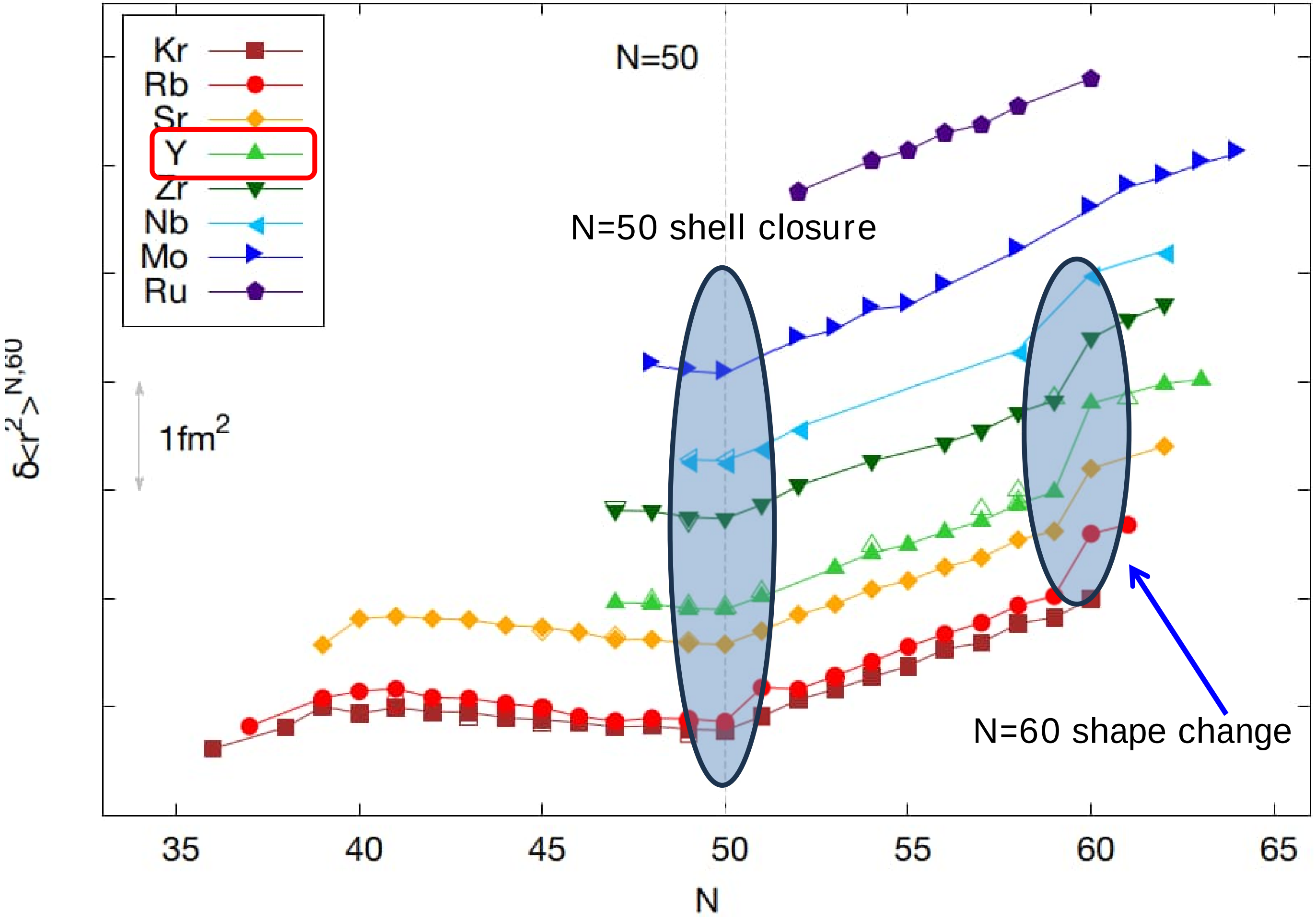
Lower *Z* requires high resolution techniques

Higher *Z* lower resolution methods

From the isotope shift to the nuclear size

Raw data: optical spectra of Y isotopes





N=50 shell closure

N=60 shape change

More about the nuclear size and nuclear structure tomorrow!

Properties of a (radioactive) nucleus

Weight

Size

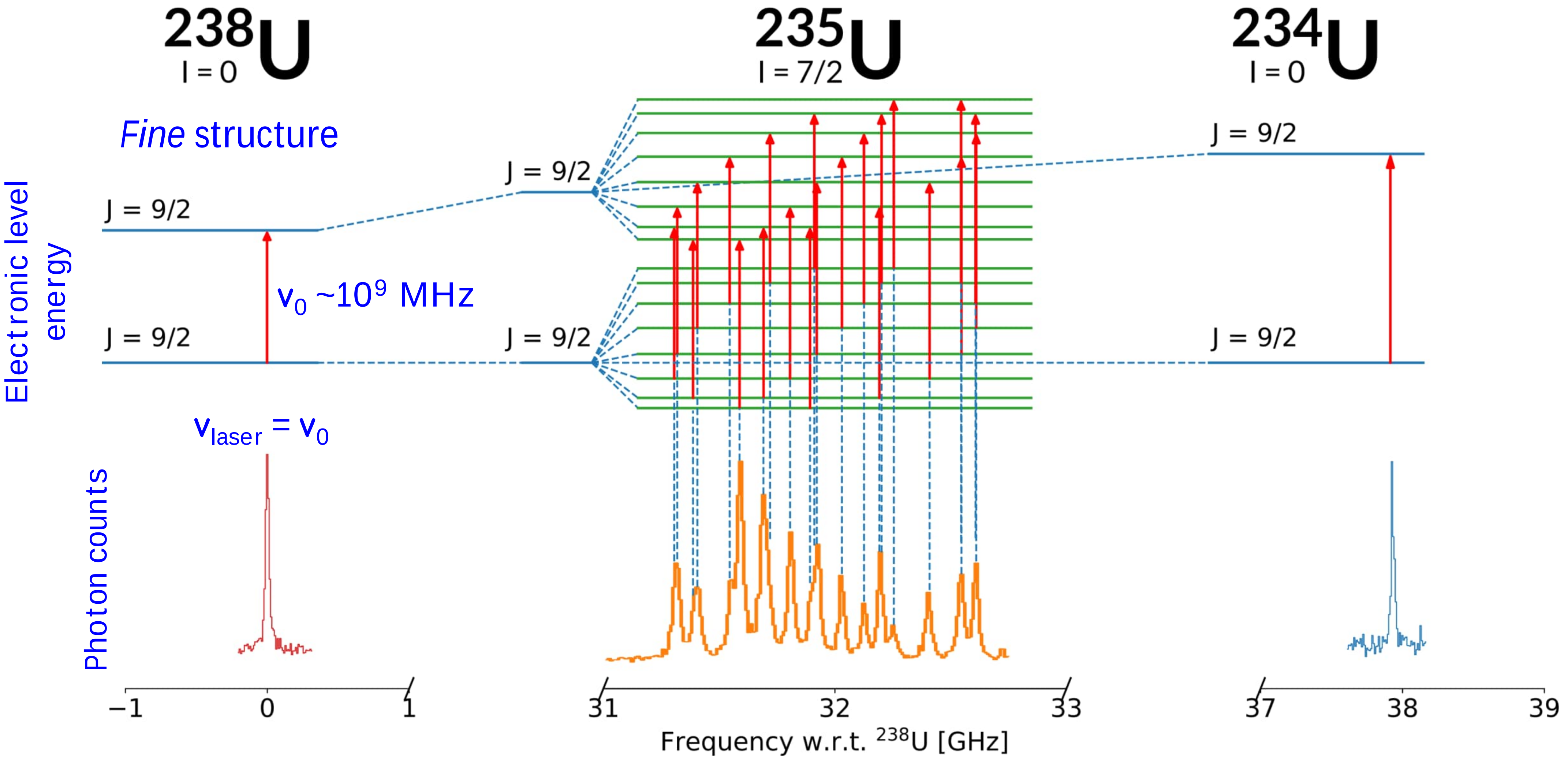
Lifetime/decay

Shape

Electromagnetic property

Is it excited or not?

Let’s return to the atomic structure of uranium…



Hyperfine interaction (in free atoms)

Hyperfine interaction = the interaction of nuclear magnetic and electric moments with electromagnetic fields (which are produced at the nucleus by the orbiting electrons)

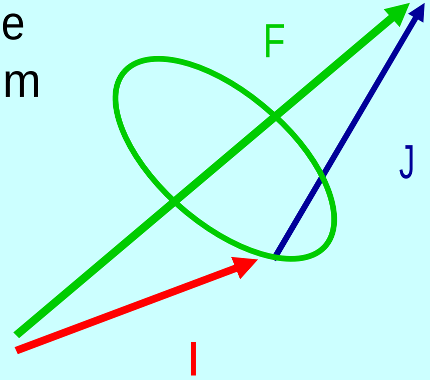
Lets consider the effect on an atomic orbit of spin J (where J = L + S) – our fine structure orbital.

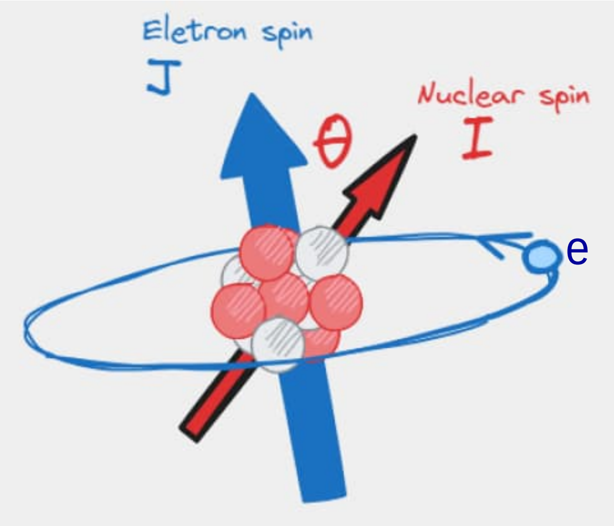
The atomic and nuclear spins couple to form the total angular momentum

F = I + J

Each state J has several F-states:

$$\vec{F} = \vec{I} + \vec{J}$$





$$F = I + J, I + J - 1, \ldots, |I - J|$$

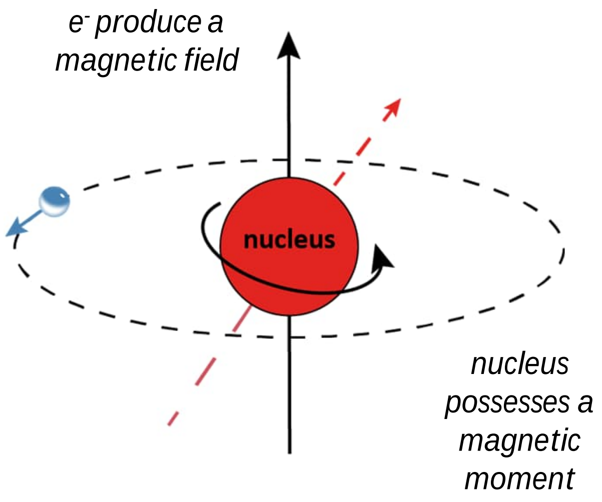
States of the same I and J but coupled to different angular momenta F have slightly different energies

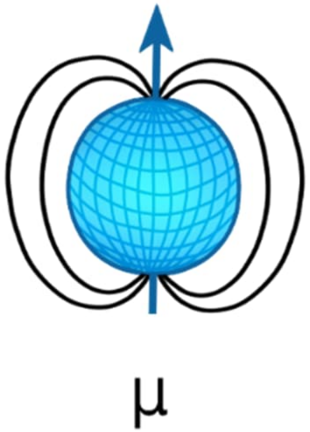
Nuclear magnetic dipole moment

From the definition:

$$\hat{\mu}_I = \sum_i \left(g_l^i \mathbf{l_i} + g_s^i \mathbf{s_i}\right) = g\mathbf{I}\mu_N$$

We can see there are contributions from orbiting charge and intrinsic spin





Protons:	$g_l = +1$	$g_s = +5.586$
Neutrons:	$g_l = 0$	$g_s = -3.826$

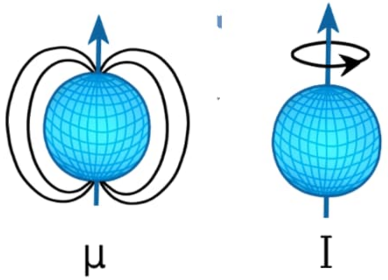
(These are values for a *free* proton/neutron)

The magnetic dipole moment of a state of spin I = expectation value of the z-component of the dipole operator μ:

$$\mu(I) \equiv \left\langle I, m = I \middle| \hat{\mu}_z \middle| I, m = I \right\rangle = gI\mu_N$$

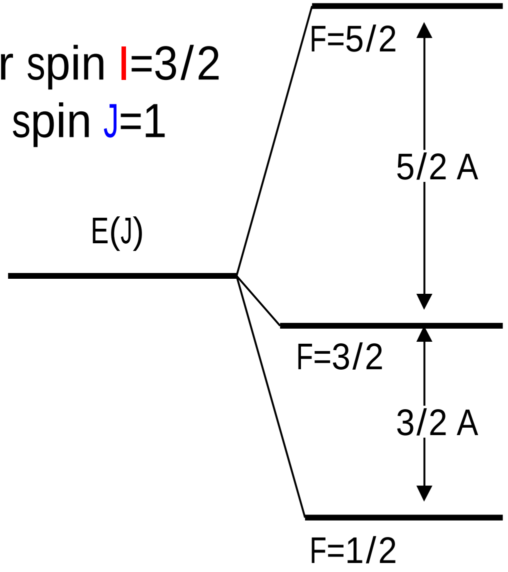
Measuring a magnetic moment is an excellent way to learn more about the wavefunction/configuration of the nucleus.

The magnetic dipole interaction



^{201}Hg

Nuclear spin I=3/2
Atomic spin J=1

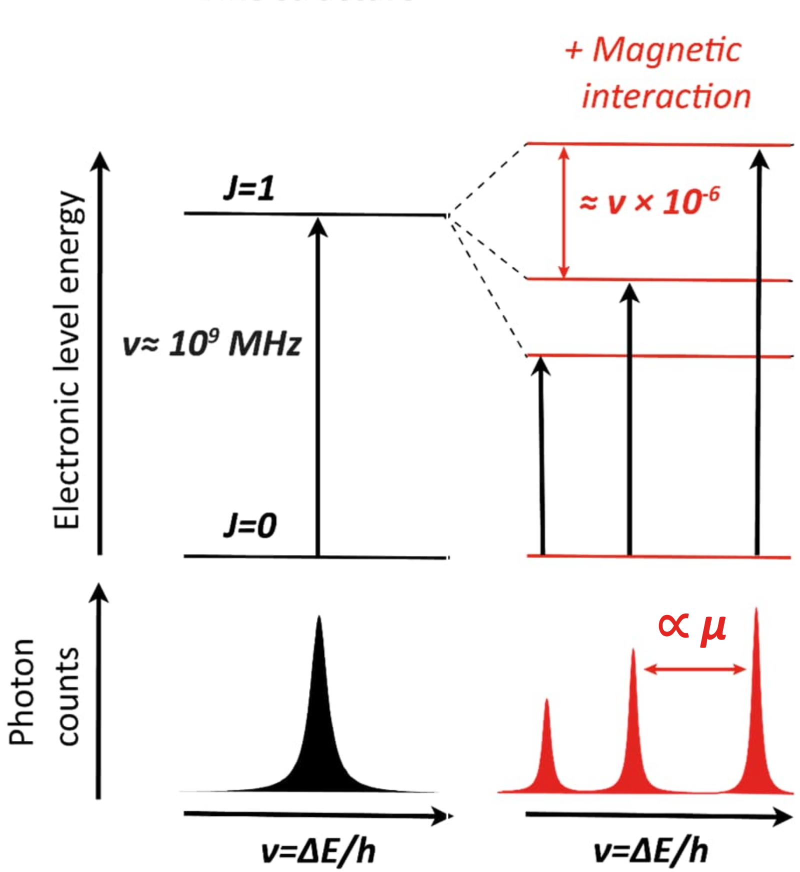


The interaction energy depends on angle θ

$$E = -\boldsymbol{\mu}\cdot\mathbf{B}_e = -\mu B_e \cos\theta$$

$$A = \frac{\mu_I B_e(0)}{I\cdot J},$$

$B_e(0) =$ magnetic field at nucleus



The original fine structure level E(J) is perturbed so that the final energy due to the magnetic hyperfine effect:

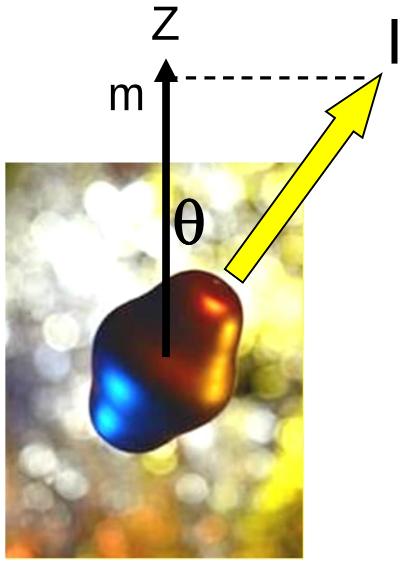
$$E(F) = \frac{A}{2}C$$

where $C = F(F+1) - I(I+1) - J(J+1)$

Access to nuclear spin I (number of hyperfine components) and μ_I

The electric quadrupole moment

The electric quadrupole moment provides a measure of the deviation of charge distribution from sphericity:



$$eQ = \int_0^\infty \rho_n(\mathbf{r})(3z^2 - r^2)\,\mathrm{d}\tau$$

A spherical nucleus would have zero Q

Experiments measure the maximum ”projection” of the intrinsic quadrupole moment along the quantization axis

Using angular momentum algebra, we get

$$Q_s = Q_0 \frac{3K^2 - I(I+1)}{(I+1)(2I+3)}$$

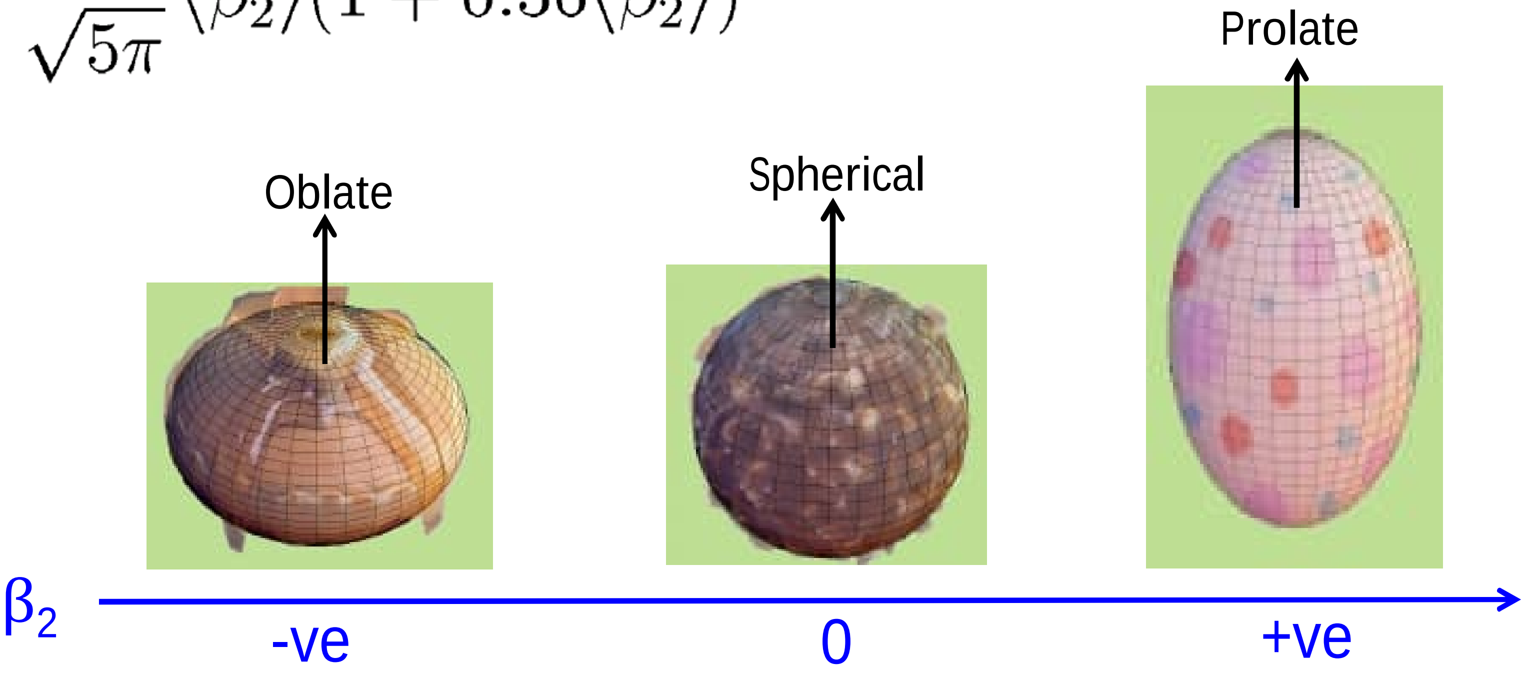
this assumes a well-defined deformation axis (not always a good approximation)

Note for nuclear spin I=0 and I=1/2 the spectroscopic quadrupole moment vanishes even if the intrinsic shape is deformed.

The electric quadrupole moment

The intrinsic Q moment can in turn be related to the quadrupole deformation parameter β_2

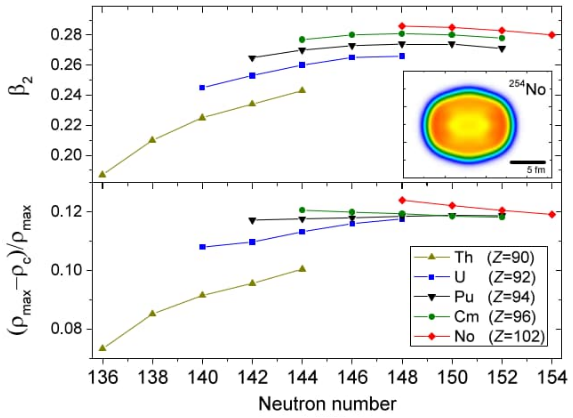
$$Q_0 \approx \frac{3Zr_0^2}{\sqrt{5\pi}}\langle\beta_2\rangle(1+0.36\langle\beta_2\rangle)$$



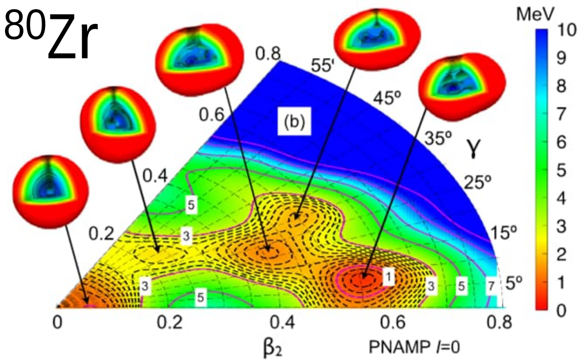
Magda will discuss more on nuclear collectivity!

Side-tracking

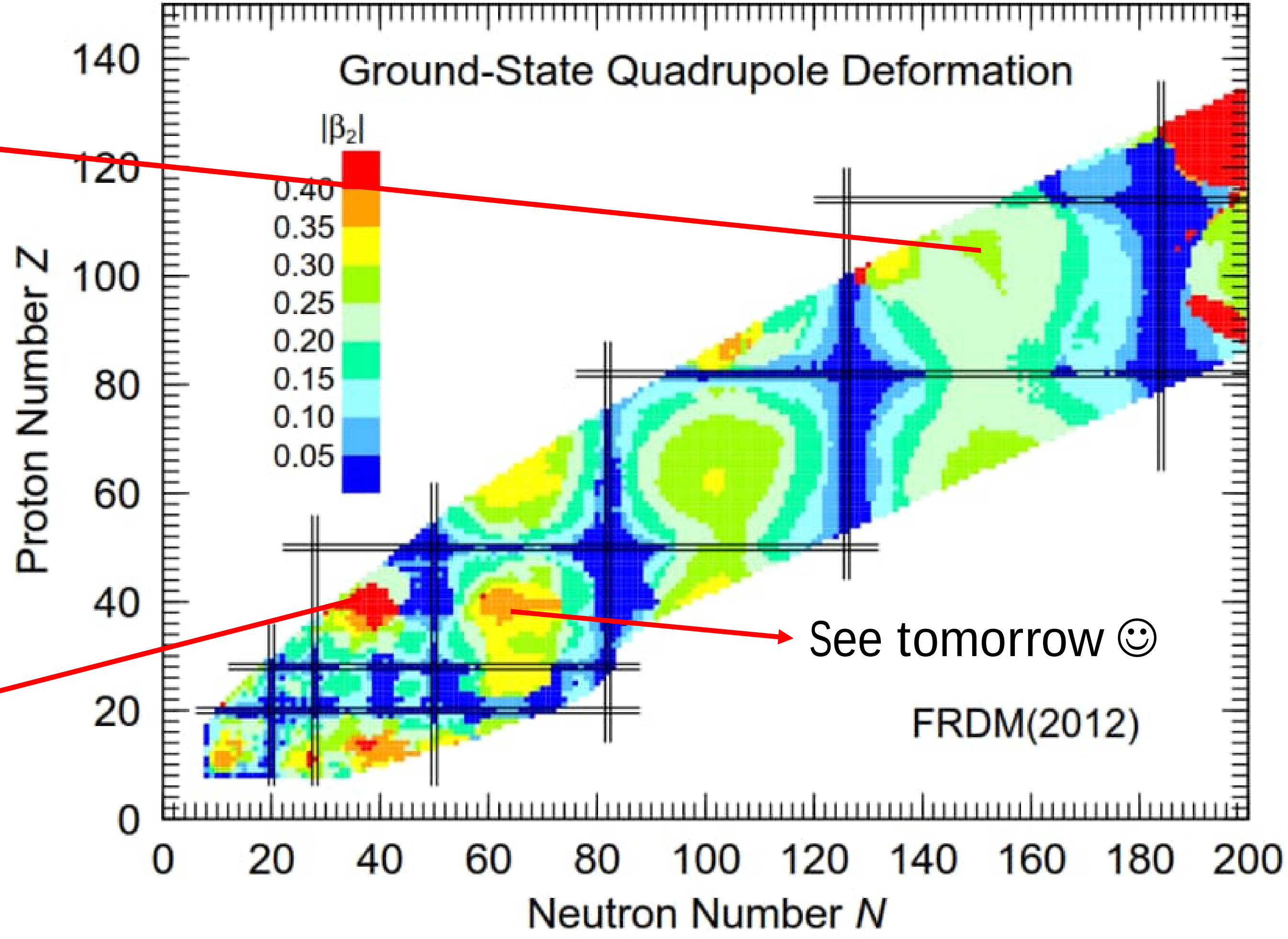
How common is quadrupole deformation? Or, how uncommon are spherical nuclei?



S. Raeder et al., PRL 120 (2018) 232503

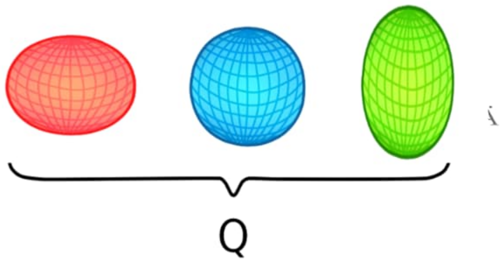


Rodriguez and Egido, PLB 705 (2011) 255



See tomorrow ☺

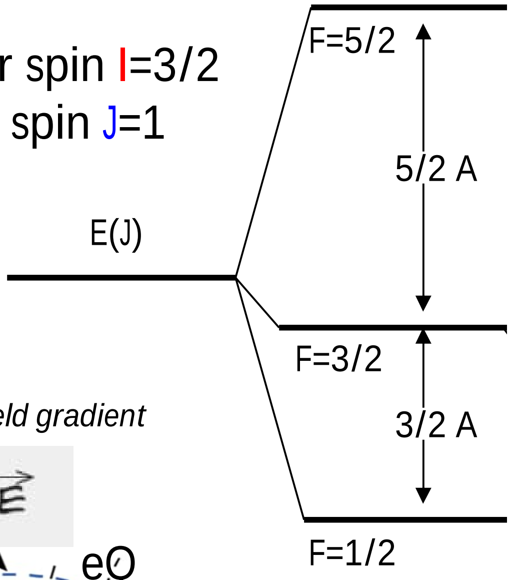
The electric quadrupole interaction



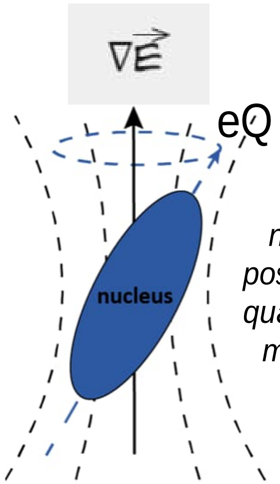
A further perturbation of the atomic level, $\propto B$

^{201}Hg

Nuclear spin I=3/2
Atomic spin J=1



Electric field gradient

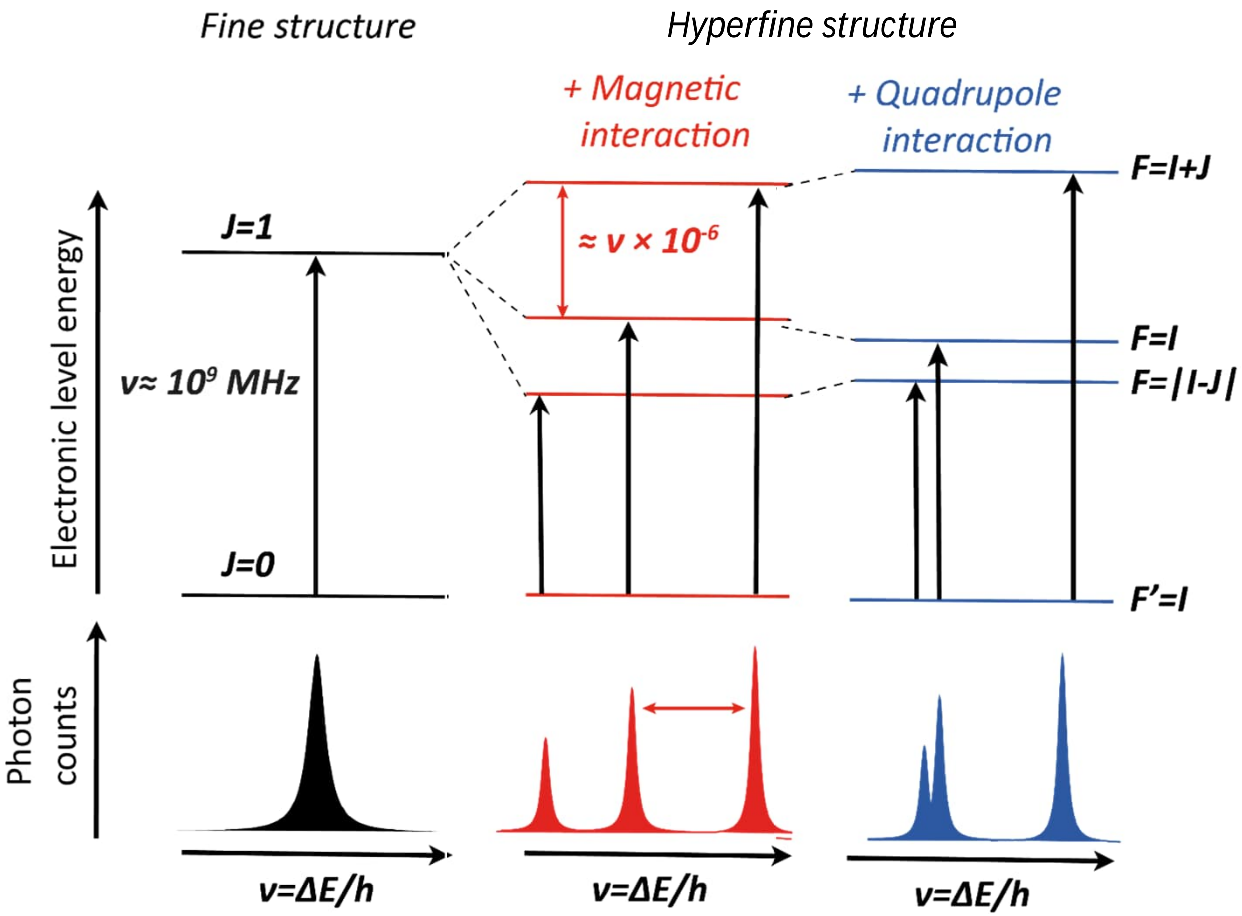


nucleus possesses a quadrupole moment

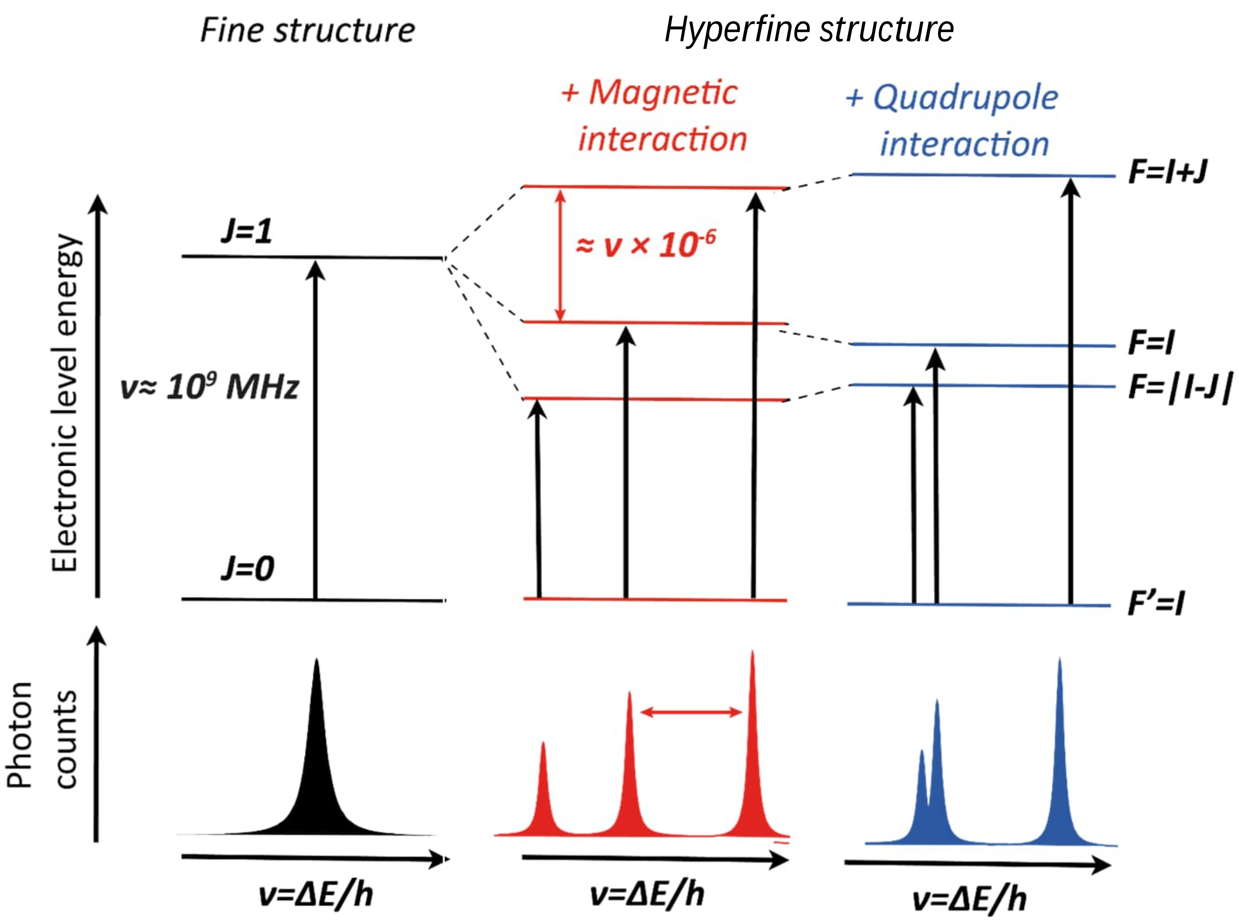
$$B = eQ_s V_{JJ}(0),$$

$$V_{JJ}(0) = \text{electric field gradient at nucleus}$$

Access to Q_s



Let’s summarize…



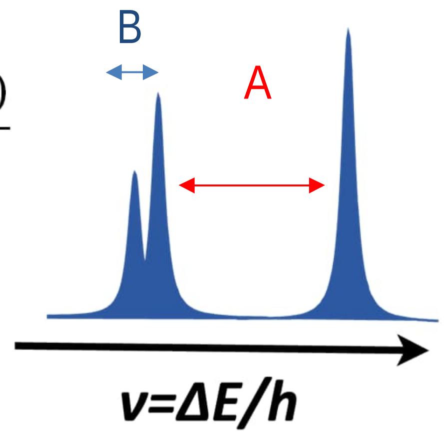
- The hyperfine interaction manifests as a splitting and perturbation of the atomic fine structure lines.
- The energy of the F state is given by:

$$E(F) = \frac{A}{2}C + B\,\frac{\frac{3}{4}C(C+1) - I(I+1)J(J+1)}{2(2I-1)(2J-1)I\cdot J} \quad +$$

$$\text{where} \quad C = F(F+1) - I(I+1) - J(J+1)$$

- Experimentally we extract the A and B hyperfine coefficients from either the upper or lower fine structure state:

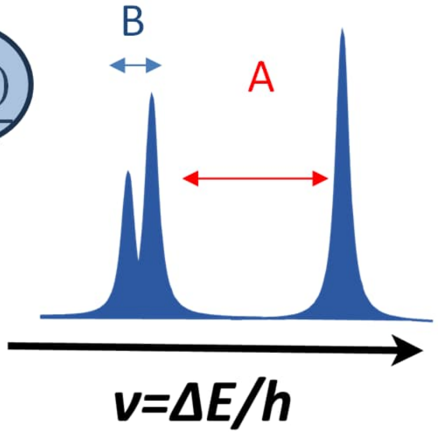
$$A = \frac{\mu_I B_J(0)}{I\,J}$$



$$B = eQ_s V_{JJ}(0)$$

In reality what we are measuring

$A = \frac{\mu_I B_J(0)}{I J}$



$B = eQ_s V_{JJ}(0)$

- To extract the hyperfine parameters A and B from experimental measurements, the magnetic field B_J and electric field gradient V_{jj} need to be extracted.
- This can be done in principle using atomic theory
- A more elegant way is to use reference nuclei with known moments. B_J and V_{jj} depend only on electronic structure.

Nuclear magnetic moment

$$\frac{A_1}{A_2} = \frac{\mu_1}{I_1}\frac{I_2}{\mu_2}$$

Reference nuclei (stable isotopes) with accurately known moments

$$\mu_1 = \frac{I_1}{I_2}\frac{A_1}{A_2}\mu_2$$

A_1, A_2 from fit
μ_2 from NMR

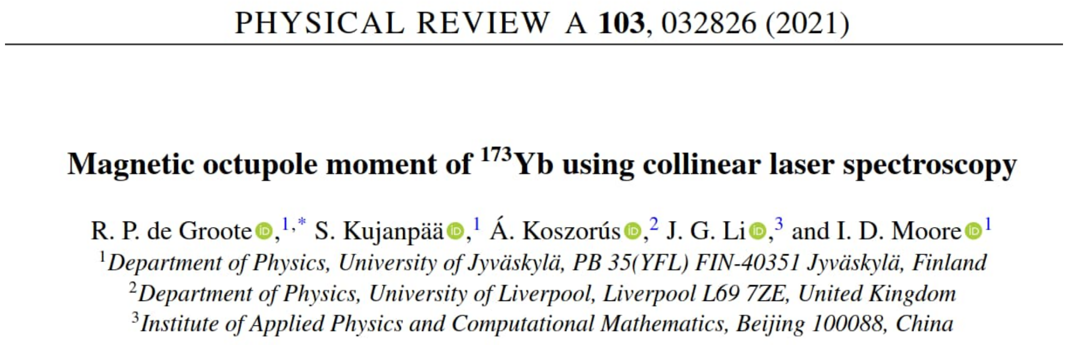
Nuclear quadrupole moment

$$B = eQV_{JJ}(0)$$

$$Q = \frac{B}{eV_{JJ}(0)}$$

B from fit
Electric field gradient from atomic physics

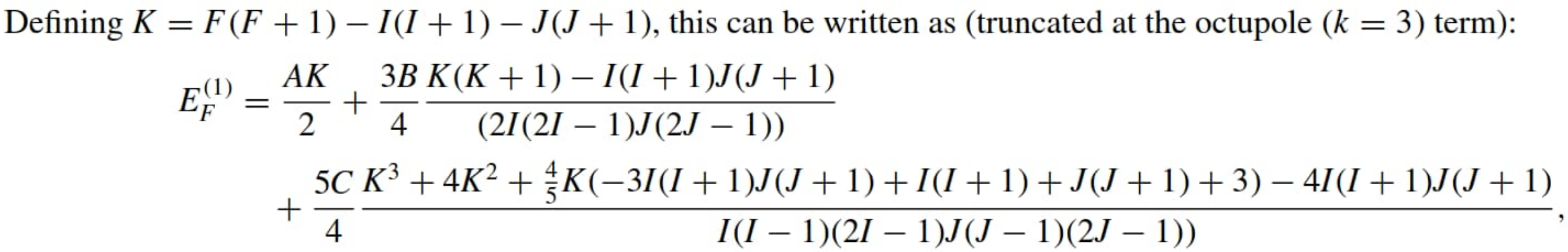
Did anyone notice the little ”+” sign 2 slides ago?



PHYSICAL REVIEW A **103**, 032826 (2021)

Magnetic octupole moment of ^{173}Yb using collinear laser spectroscopy

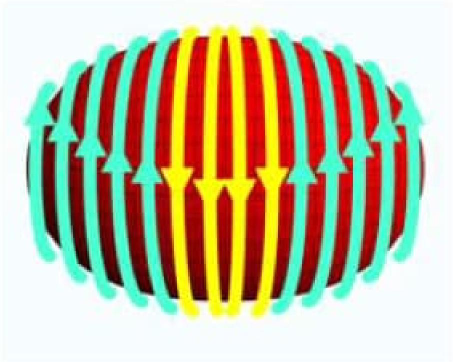
R. P. de Groote,[1,*] S. Kujanpää,[1] Á. Koszorús,[2] J. G. Li,[3] and I. D. Moore[1]
[1]*Department of Physics, University of Jyväskylä, PB 35(YFL) FIN-40351 Jyväskylä, Finland*
[2]*Department of Physics, University of Liverpool, Liverpool L69 7ZE, United Kingdom*
[3]*Institute of Applied Physics and Computational Mathematics, Beijing 100088, China*



Defining $K = F(F+1) - I(I+1) - J(J+1)$, this can be written as (truncated at the octupole ($k = 3$) term):

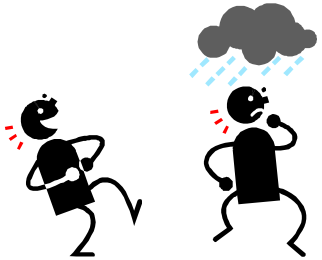
$$E_F^{(1)} = \frac{AK}{2} + \frac{3B}{4}\frac{K(K+1) - I(I+1)J(J+1)}{(2I(2I-1)J(2J-1))} + \frac{5C}{4}\frac{K^3 + 4K^2 + \frac{4}{5}K(-3I(I+1)J(J+1) + I(I+1) + J(J+1) + 3) - 4I(I+1)J(J+1)}{I(I-1)(2I-1)J(J-1)(2J-1))},$$

- Measurements of the magnetic octupole constant C and moment Ω are scarce!
- Currently only measured for about 18 elements, and all stable isotopes.
- Interpretation of such a moment is somewhat lacking and due to a lack of data, not much theoretical progress in over half a century.



Magnetic octupole

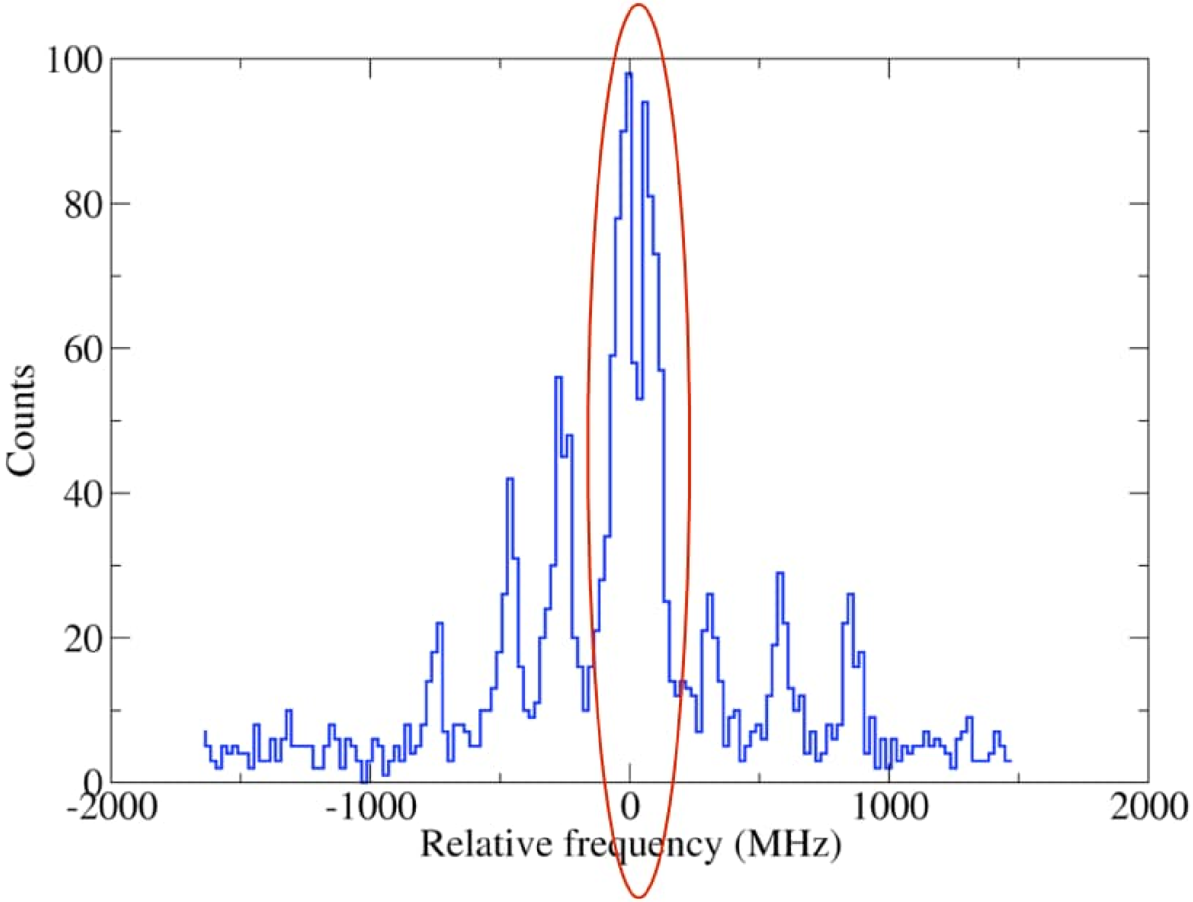
And finally – discovering nuclear states



Is it excited or not?

- It might have been too long-lived for nuclear decay spectroscopy methods
- It could have been too low-lying to be separated by precision mass measurements
- Discovered by optical spectroscopy through the hyperfine pattern!
- However – optical spectroscopy alone cannot say which state is the ground state and which is the isomer…

Example of an isomer in ^{80}Ga



Cheal *et al.* Phys. Rev. C **82**, 051302(R)

Take home messages and outlook to lecture 2

Weight

Size

Shape

Electromagnetic property

- The nuclear mass and binding energy contain a wealth of structural information, but need supported by other techniques to understand the nature of structural changes.

- The nuclear spin can be determined unambiguously in a nuclear model-independent way – e.g., counting the observed number of resonances.
  - assumes sufficient experimental resolution (L2)

- A measurement of hyperfine structure gives access to magnetic dipole and electric quadrupole moments (single particle and collective properties)

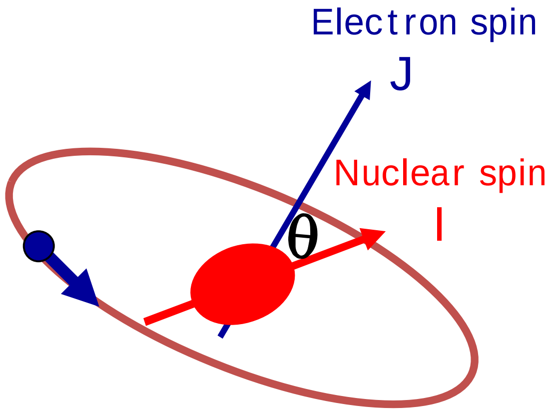
- The isotope shift is a gateway to the nuclear size (charge radii).
  - close connection with shell structure, deformation
  - complementary to information from binding energies (L2)

Back up material for lecture 1

The magnetic dipole interaction

The interaction energy depends on angle θ

$$E = -\boldsymbol{\mu} \cdot \mathbf{B_e} = -\mu B_e \cos\theta$$



Since $\boldsymbol{\mu} = g\mathbf{I}\mu_N$ and $\mathbf{B}_e = -(\frac{B_e}{J})\mathbf{J}$

then the interaction Hamiltonian can be expressed as

$$H_m = (\frac{gB_e\mu_N}{J})\mathbf{I}.\mathbf{J} = A\mathbf{I}.\mathbf{J}$$

The different energy shifts of the different F-states are then

$$\Delta E = \langle IJF \mid H_m \mid IJF \rangle = A\langle \mathbf{I}.\mathbf{J} \rangle$$

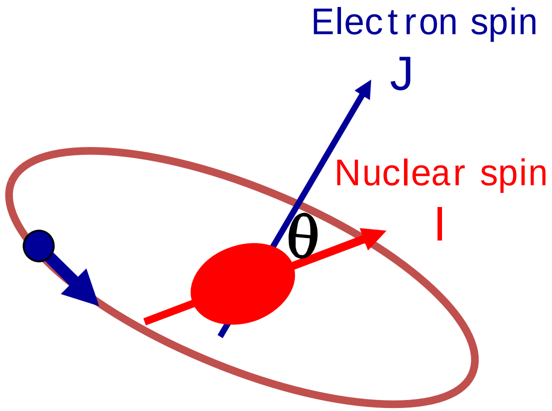
Where:

$$\langle \mathbf{I}.\mathbf{J} \rangle = \frac{1}{2}\langle F^2 - I^2 - J^2 \rangle = \frac{1}{2}[F(F+1) - I(I+1) - J(J+1)]$$

The electric quadrupole interaction

$$E = \tfrac{1}{4}\, e\, Q_0\, V_{JJ}\, P_2(\cos\theta)$$

Electric field gradient along J-direction due to atomic electrons.



Energy shifts of the F-states are then

$$\Delta E_Q = \frac{B}{4}\frac{\frac{3}{2}C(C+1) - 2I(I+1)J(J+1)}{I(2I-1)J(2J-1)}$$

Where: $C = [F(F+1) - I(I+1) - J(J+1)]$

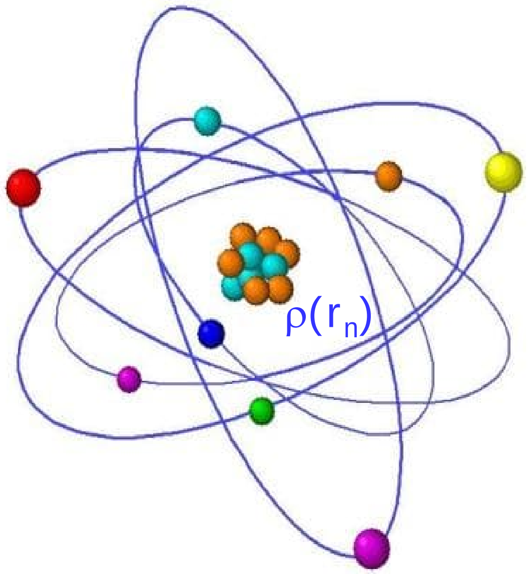
The hyperfine factor “B” is measured by experiment: $B = eQ_s\langle\frac{\partial^2 V}{\partial Z^2}\rangle = eQ_sV_{JJ}$

The electric field gradient V_{JJ} may be calibrated with an isotope with known Q_s

The nuclear charge distribution

Expanding the charge distribution in multipoles:

$$Q_q^n = eZ\sqrt{\frac{4\pi}{2n+1}}\langle I | r_n^n Y_q^n(\theta_n,\varphi_n) | I \rangle$$



- Electric monopole = $eZ\sqrt{4\pi}\langle I | Y_0^0 | I \rangle = eZ$
- Electric dipole = $eZ\sqrt{\frac{4\pi}{3}}\langle I | r\, Y_q^1 | I \rangle$ = 0
- Electric quadrupole: $\boxed{Q_q^2 = eZ\sqrt{\frac{4\pi}{5}}r^2 Y_q^2}$

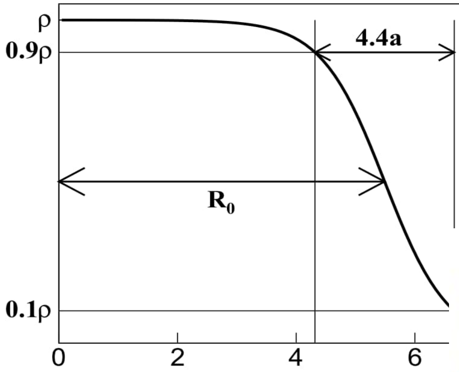
Charge radii: back to basics

The majority of modern day experiments apply electromagnetic probes to obtain (absolute) nuclear radius information – preferably point-like, e.g., electrons and muons.

The mean-square charge radius can be defined as:

$$\langle r^2 \rangle = \frac{\int r^2 \rho_{ch}(r) dV}{\int \rho_{ch}(r) dV}$$

where $\rho_{ch}(r)$ is the nuclear charge density distribution.



$$\rho_C(r) = \rho/(1 + e^{(r-R)/a})$$

Extensive studies of stable nuclei with electron scattering experiments revealed the charge density to be nearly constant in the nuclear volume.

The trend of the mean-square charge radii has the form:

$$\langle r^2 \rangle = \frac{3}{5}(r_0 A^{\frac{1}{3}})$$

Thus the rms charge radius $R = \sqrt{\langle r^2 \rangle}$ was seen to scale with $A^{\frac{1}{3}}$

Great! So we can all go home…..however….

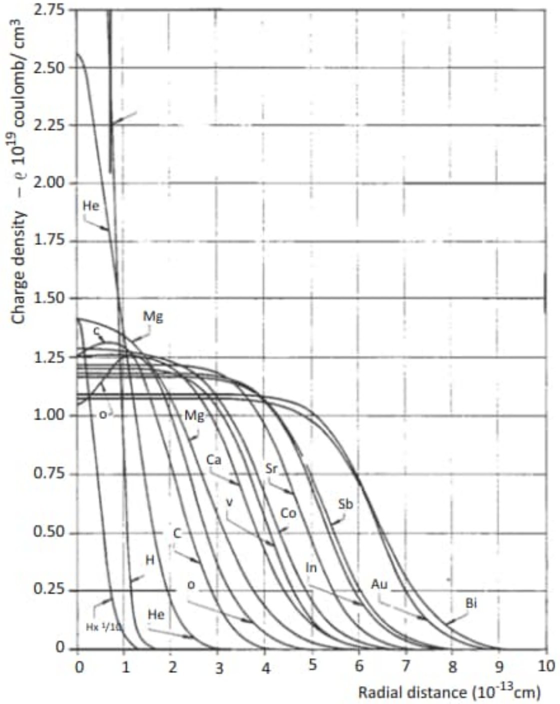
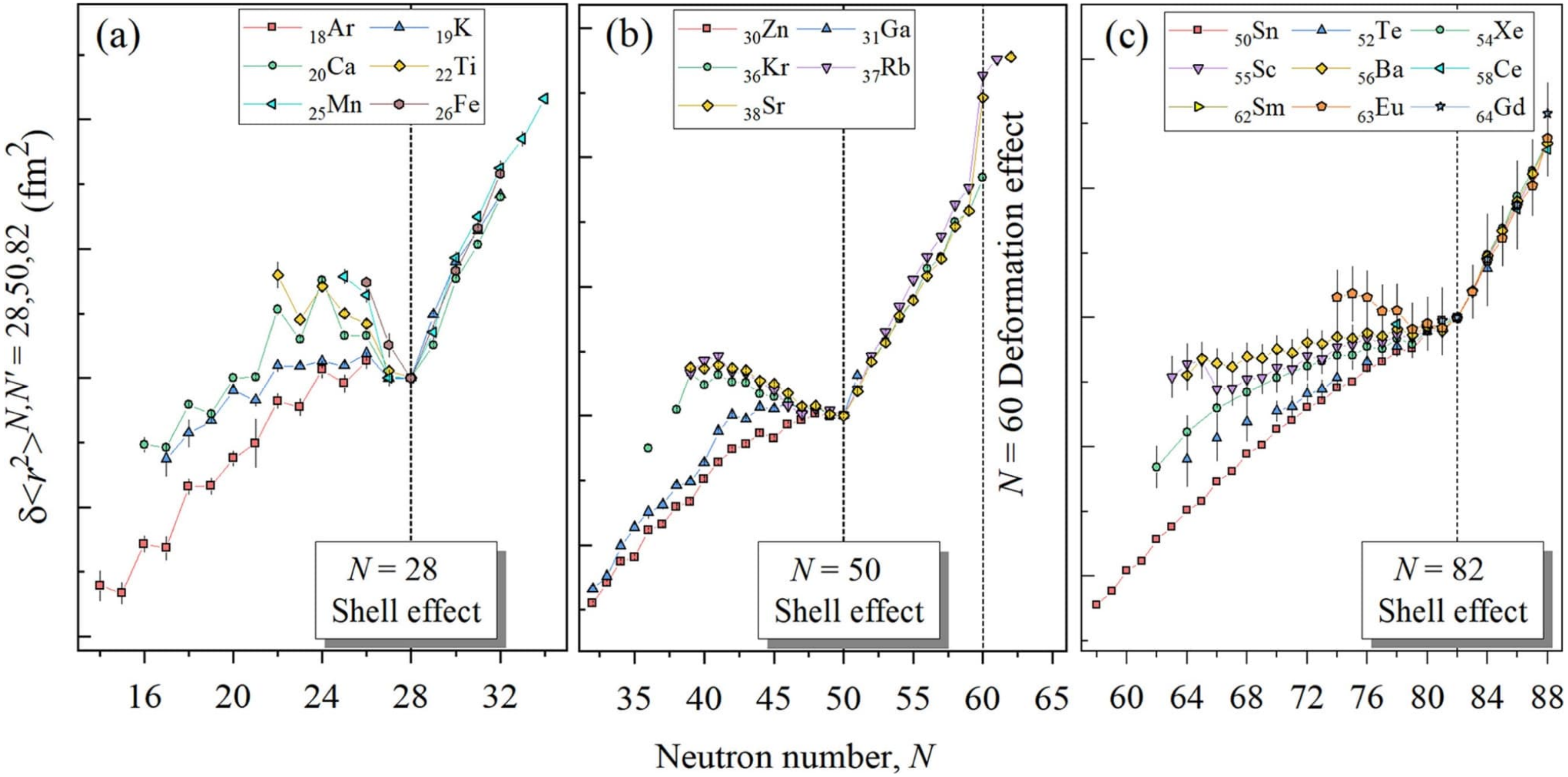
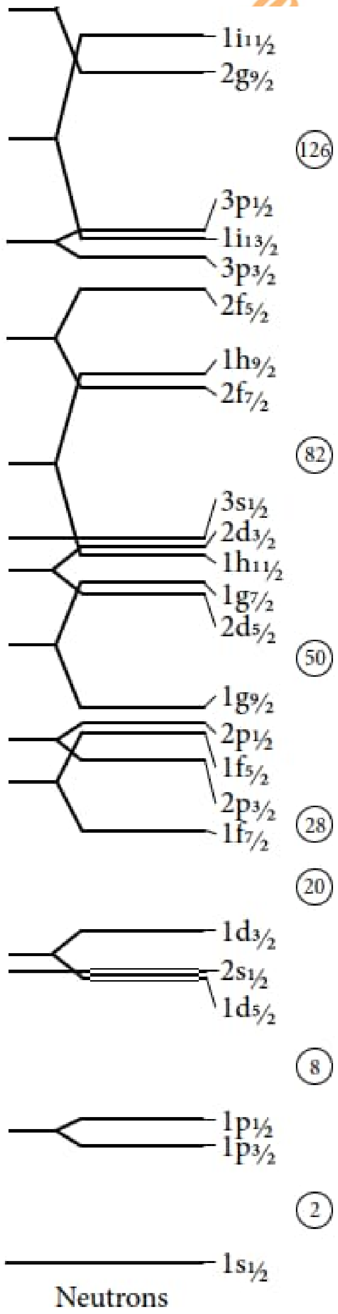


Figure from Hofstadter Nobel Prize lecture, 1961.

Nuclear shell effects - ``kinky´´ trends!





- The effect of all neutron shell closures for N≥28 is visible as a kink in the charge radii
- Much theoretical effort employed, including ab initio and DFT approaches
- Odd-even staggering effects are probed via isotope shift measurements.