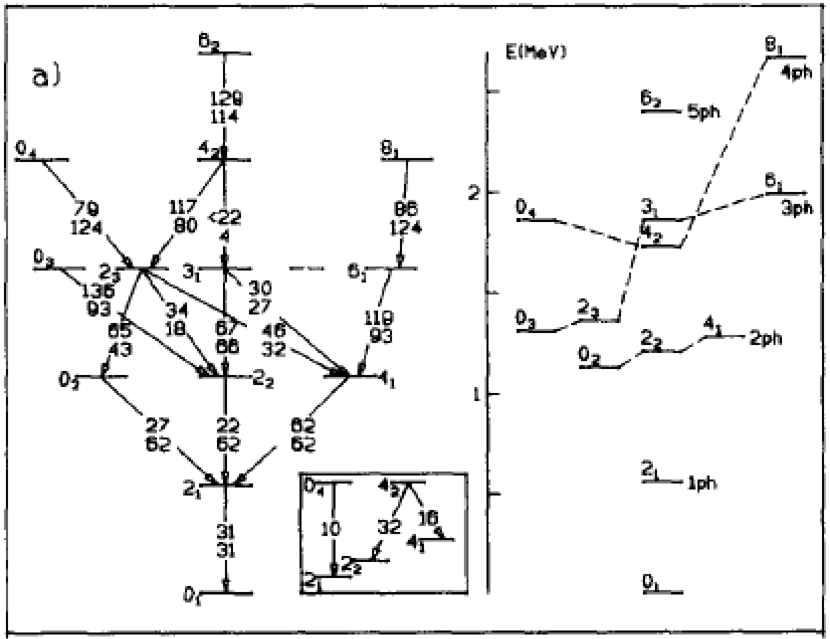
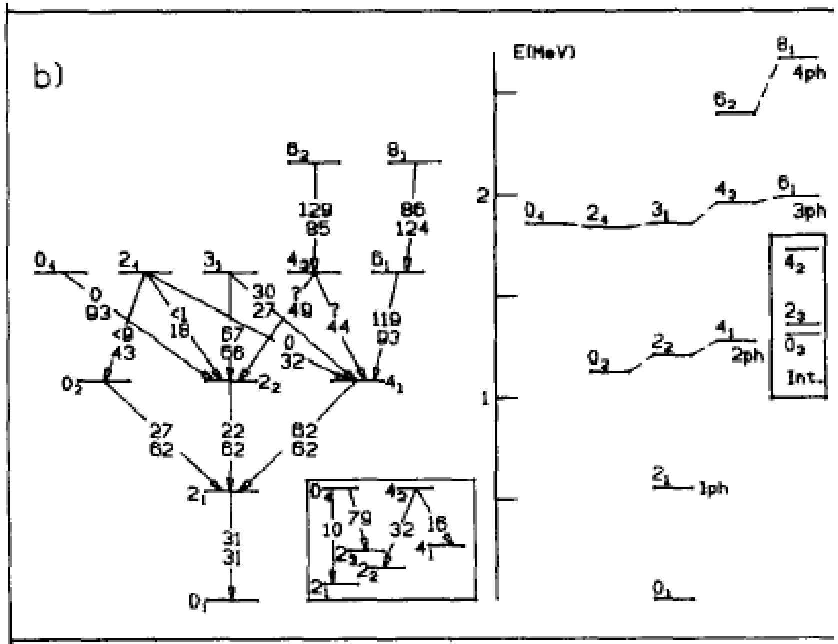
Testing Theories
(What to do and what definitely not to do)

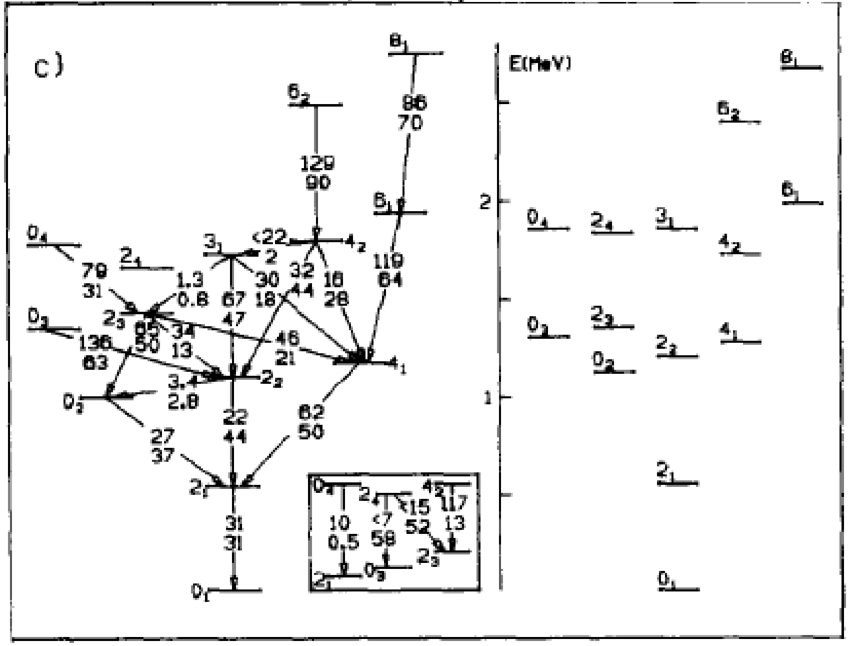
R. F. Casten
Yale

August 2014

Which theory and how to test it?







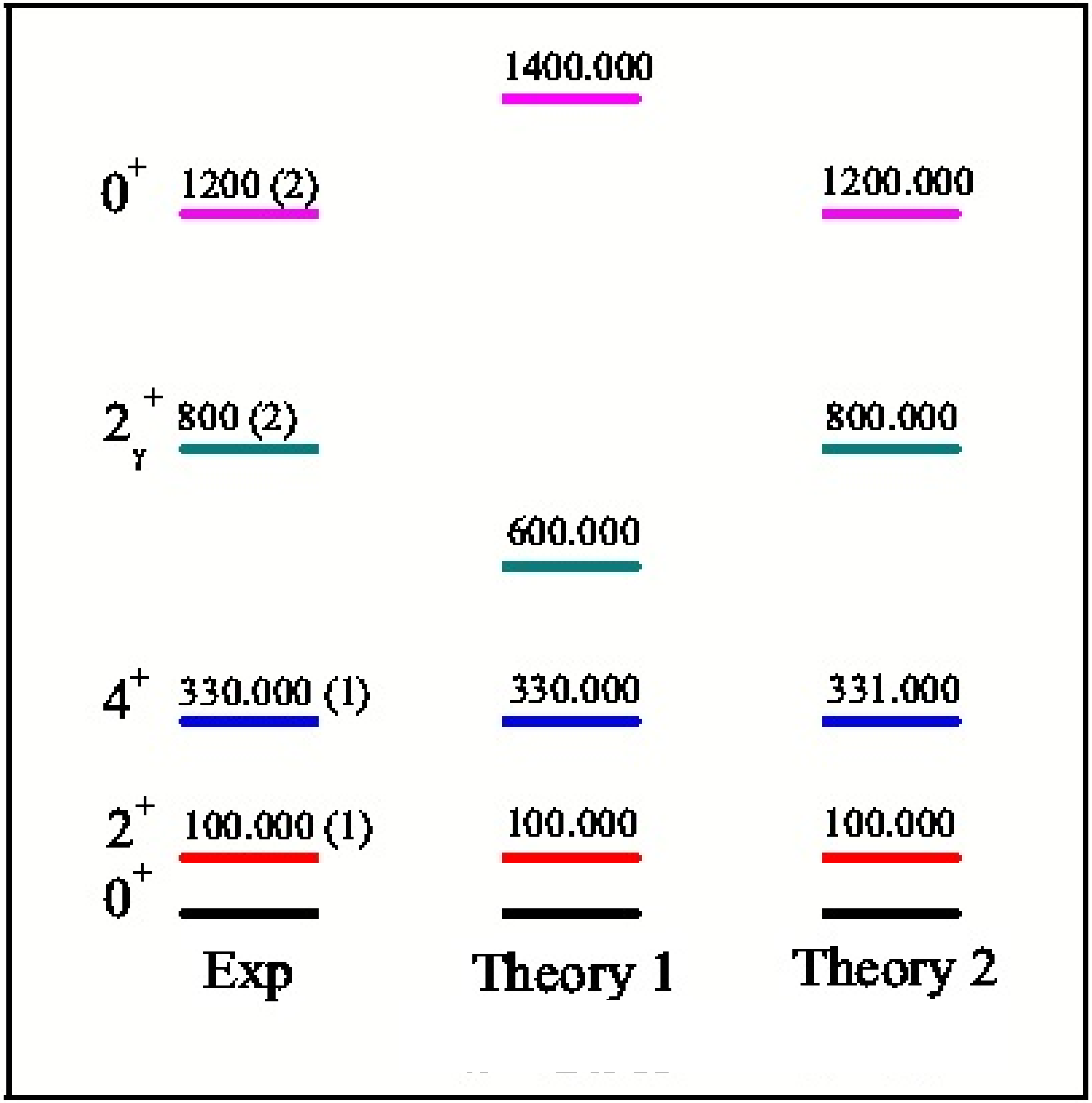
^{114}Cd

$$\chi^2 = \sum_{i=1}^{k} \left(\frac{O_i(exp) - O_i(theor)}{\sigma_i}\right)^2$$

?

A very simple first example:

Which theory is better



Now look at χ^2

$$\chi^2 = \sum_{i=1}^{k} \left(\frac{O_i(exp) - O_i(theor)}{\sigma_i} \right)^2$$

Ironically,
super-precise data can lead you astray

χ^2 analyses

$$\chi^2 = \sum_{i=1}^{k} \left(\frac{O_i(exp) - O_i(theor)}{\sigma_i} \right)^2$$

The good, the bad, and the ugly

Avoid over-weighting super-precise data

BUT

The real problem in the above example is not the accurate data per se for some states but the lack of inclusion of

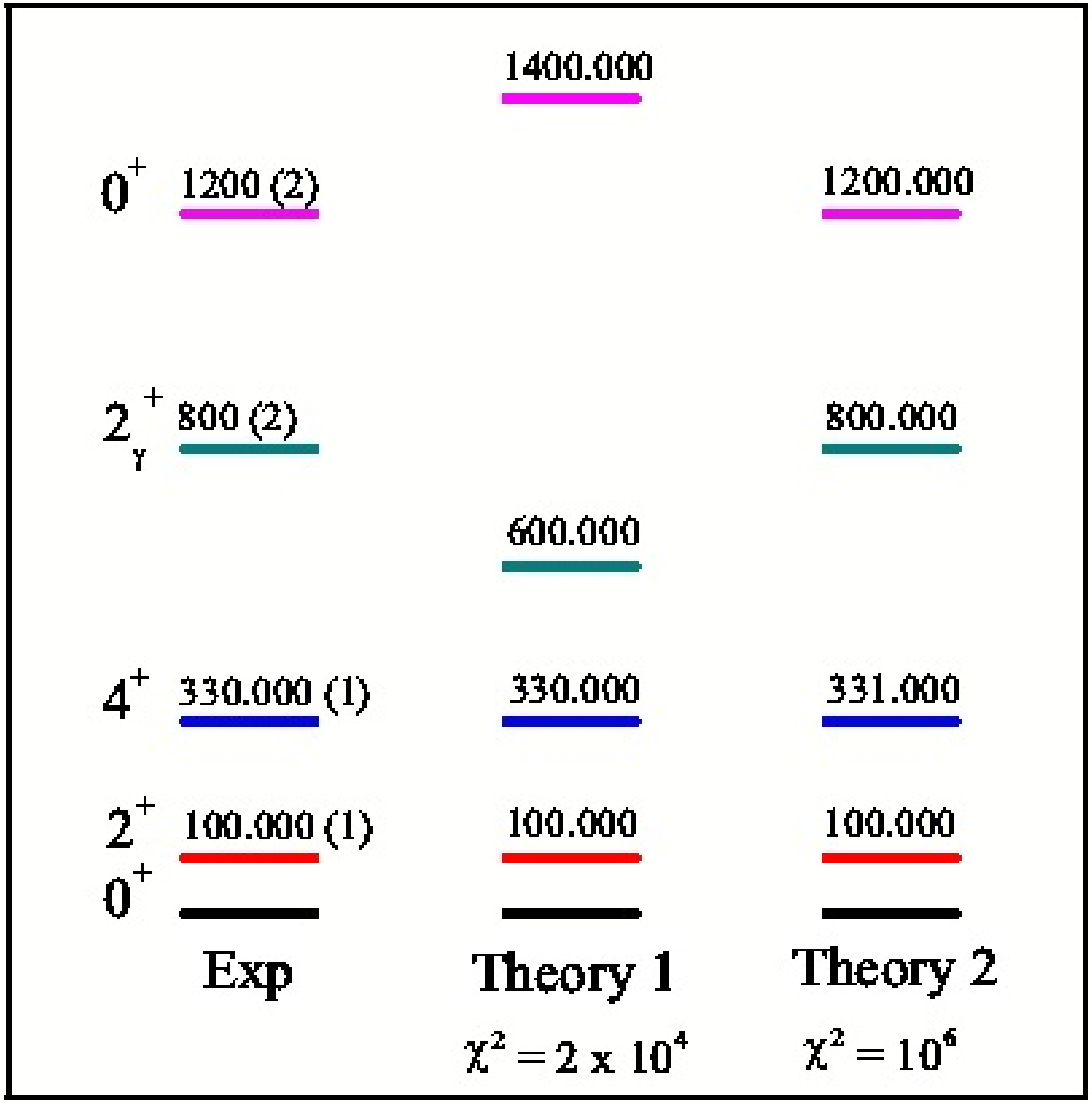
Theoretical Uncertainties

Theoretical uncertainties

This seldom refers to numerical uncertainties in the calculations but to how good we can expect a model to be.

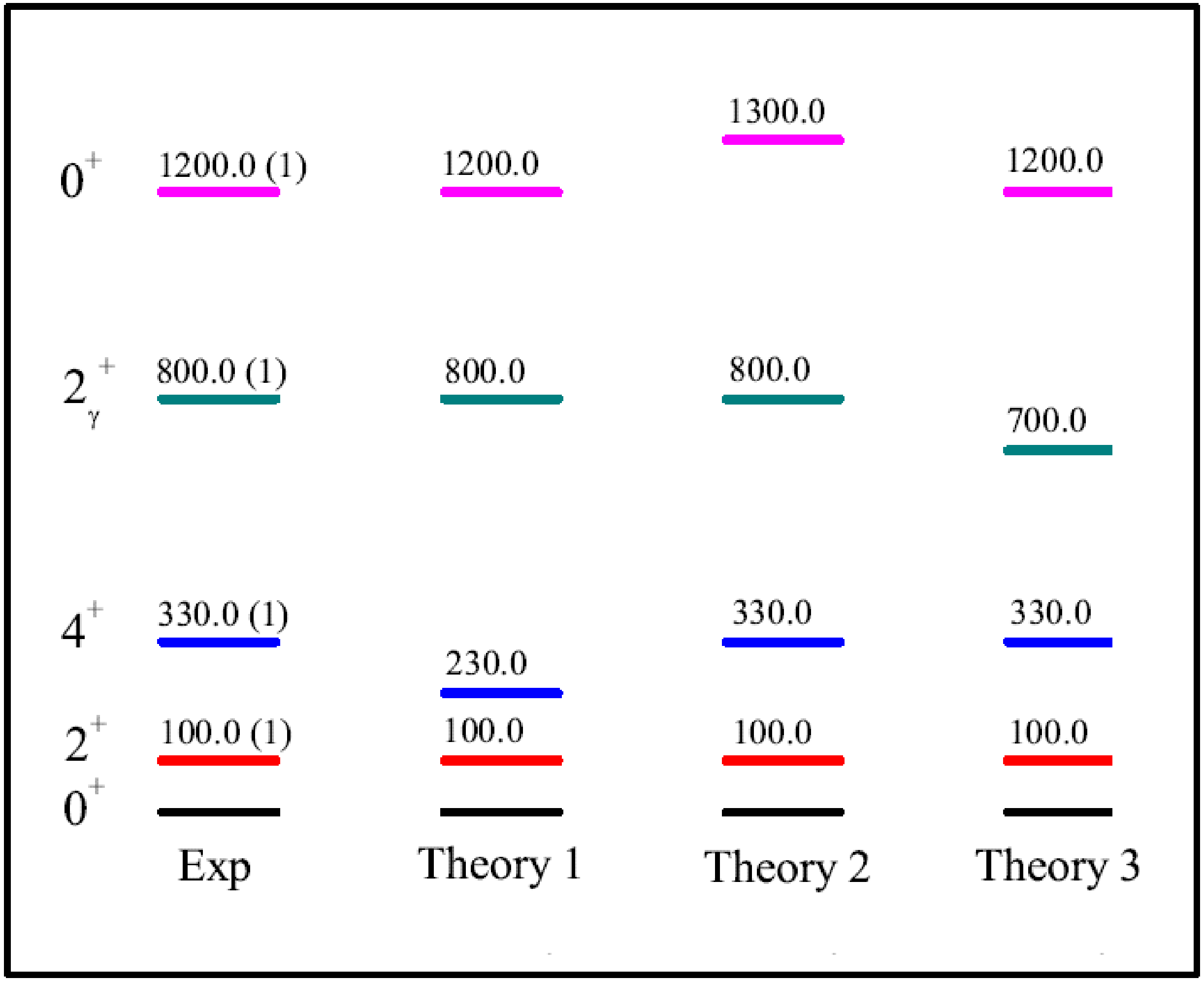
A model that says nuclei are all shaped like coca cola bottles is less likely to be accurate than one that says some nuclei are shaped like soft ellipsoids.

$$\sigma_i^2 = \sigma_i(\mathrm{exp})^2 + \sigma_i(\mathrm{Theor})^2$$


1400.000
0^+
1200 (2)
1200.000
2_γ^+
800 (2)
800.000
600.000
4^+
330.000 (1)
330.000
331.000
2^+
100.000 (1)
100.000
100.000
0^+
Exp
Theory 1
Theory 2
$\chi^2 = 2 \times 10^4$
$\chi^2 = 10^6$

~ 800 ~ 0.01

Evaluating theories with equal discrepancies



Theoretical uncertainties: Yrast: Few keV ; Vibrations ~ 100 keV

χ^2 ~1000 1

How did we estimate the theoretical uncertainties?

More or less by "feeling", experience, "communal wisdom". I would guess that most nuclear structure physicists over about 40 years old would come to similar estimates.

BUT

Its hardly rigorous and somewhat uncomfortable. Can we do better?

Answer is yes, but with a lot of work and probably not in a simple case like this. You can do a correlation analysis of theoretical/experimental deviations and get quantitative measures of the sensitivity to each observable. Gets pretty formal. See article:

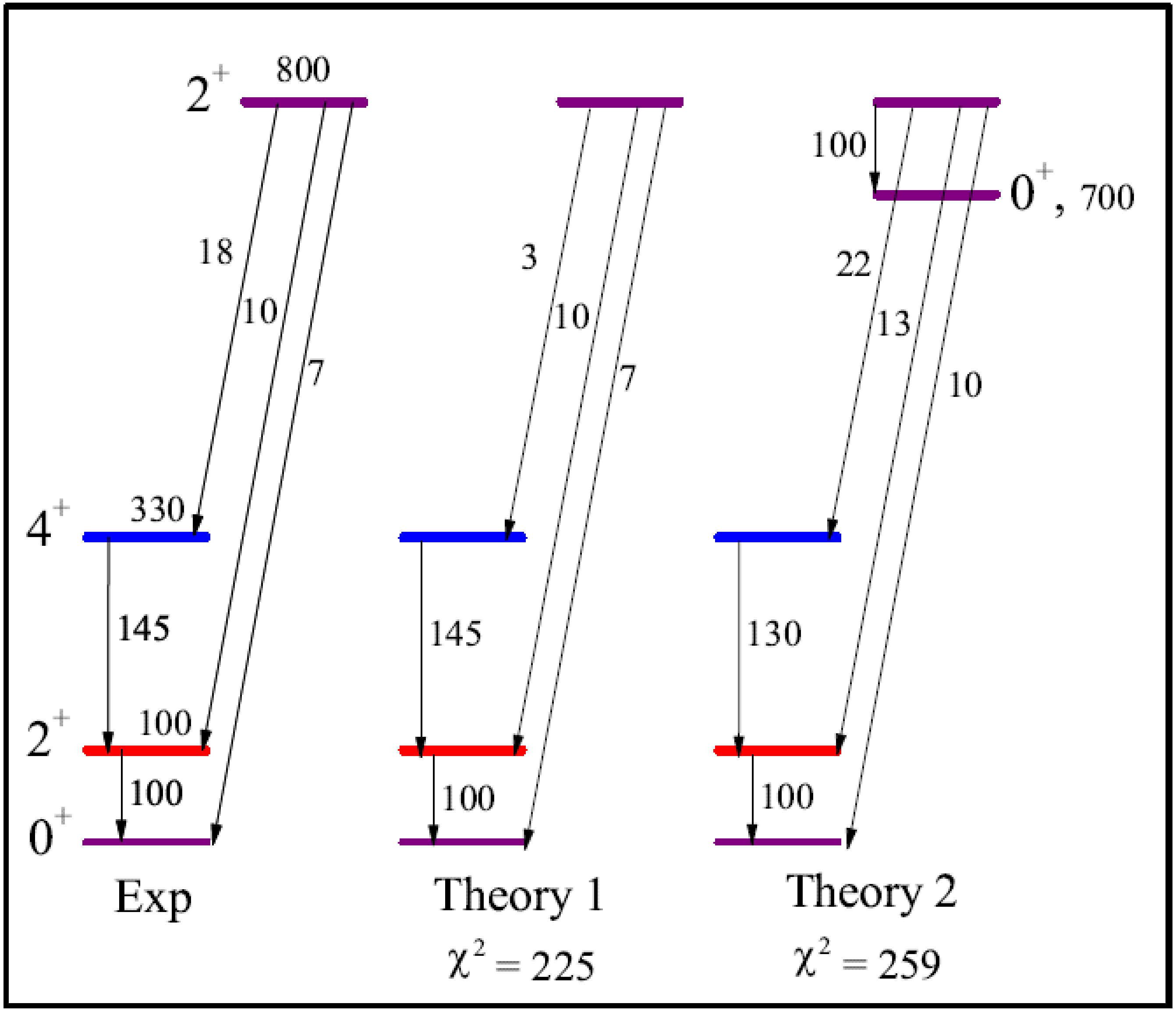
Dobaczewski J, Nazarewicz W, and Reinhard P-G 2014 *J.Phys. G* 41 074001

Also interesting for model reliability in policy making:

Saltelli A and Funtowicz S 2013 *Issues in Science and Technology Fall 2013*

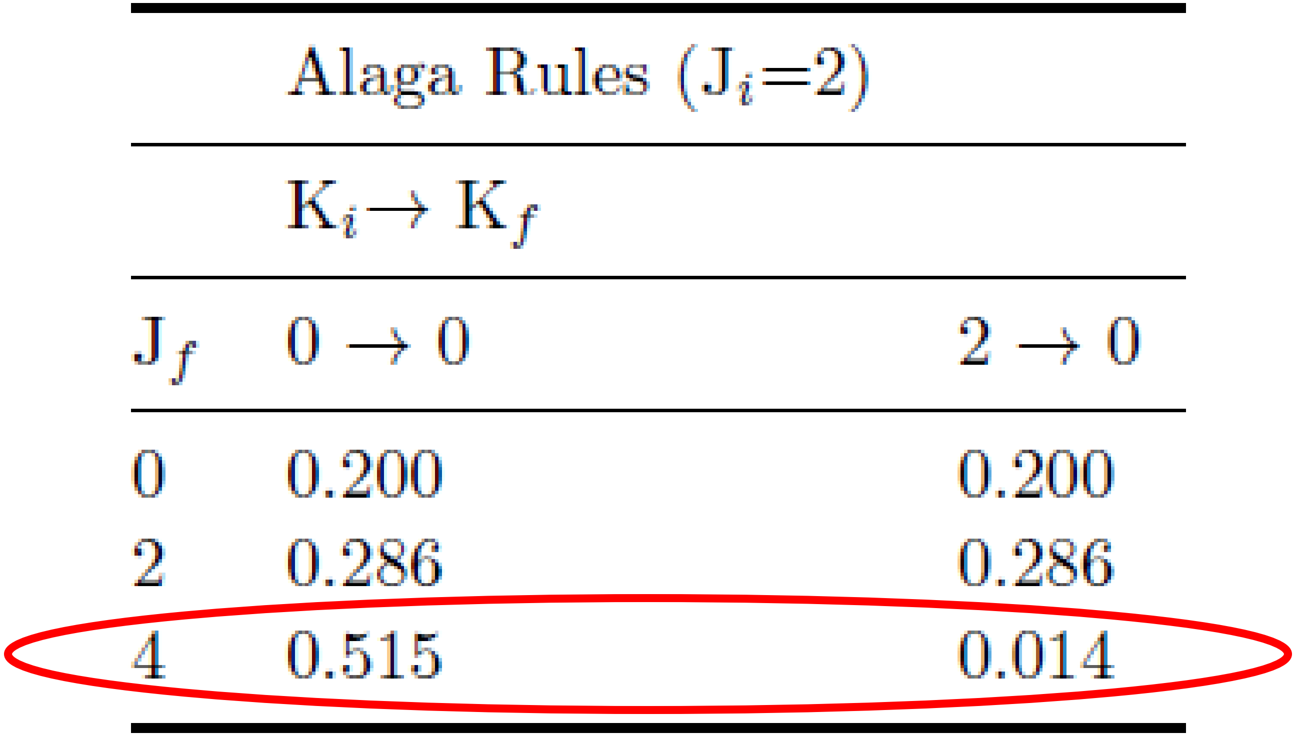
Example with B(E2) values

All exp. uncertainties 1 Wu



Here we directly use physics understanding to evaluate theories

Alaga rules



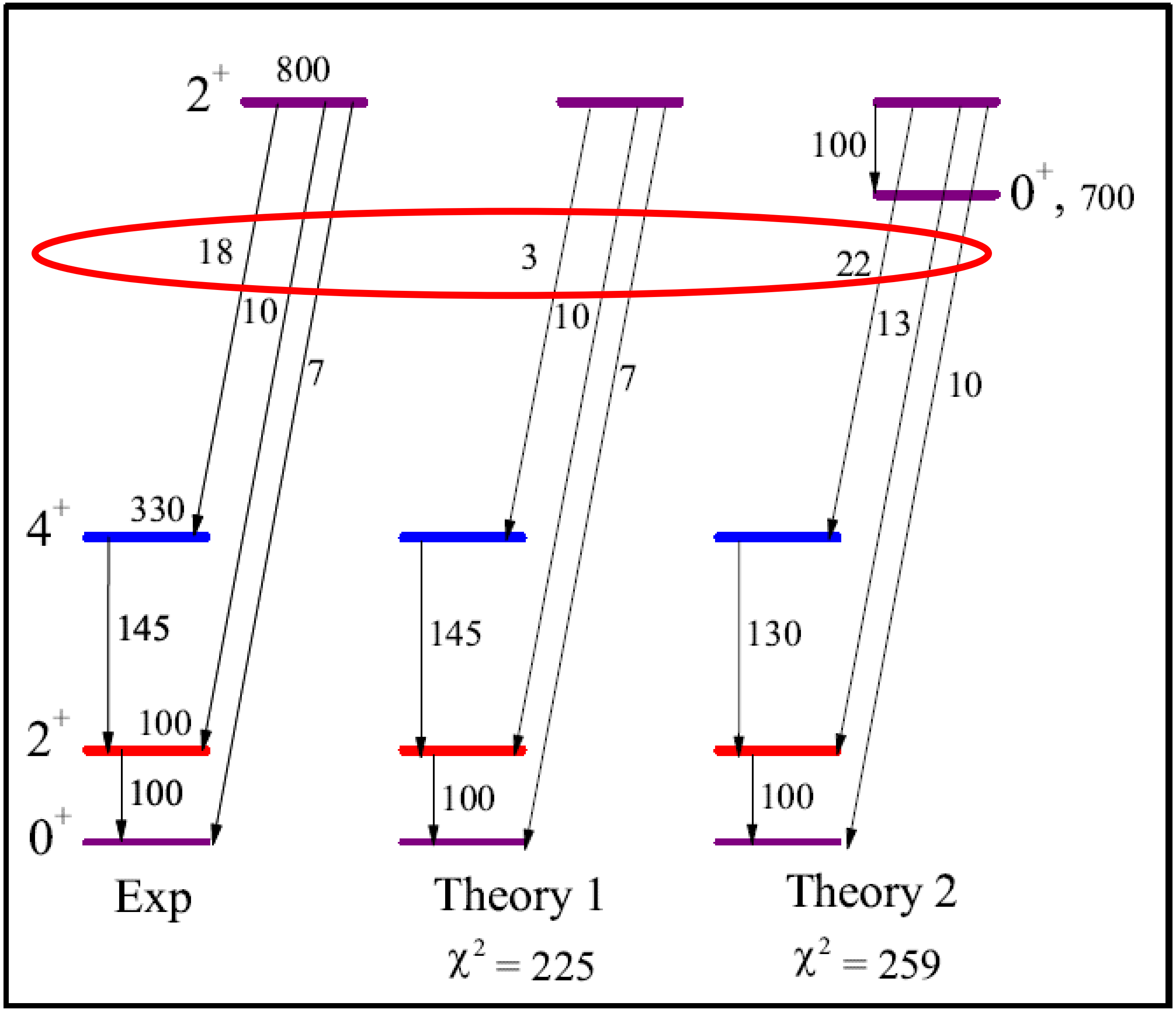
	Alaga Rules (J_i=2)	
	$K_i \to K_f$	
J_f	$0 \to 0$	$2 \to 0$
0	0.200	0.200
2	0.286	0.286
4	0.515	0.014

Transition to J = 4: **Largest** **Smallest**

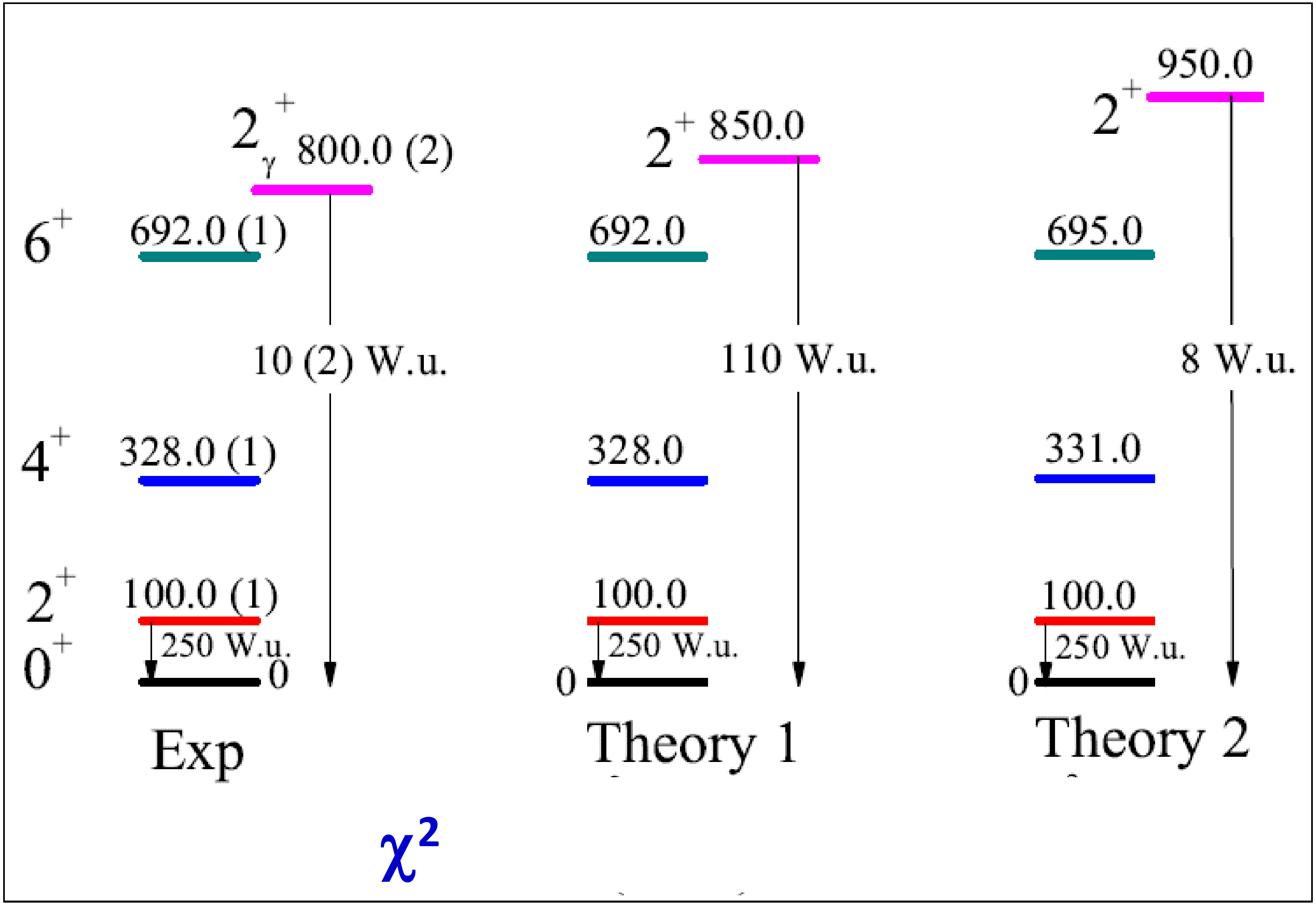
	Alaga Rules (J_i=2)	
	$K_i \rightarrow K_f$	
J_f	$0 \rightarrow 0$	$2 \rightarrow 0$
0	0.200	0.200
2	0.286	0.286
4	0.515	0.014

K = 0

with unknown 0^+



Both energies and B(E2) values



Theor. Uncertainties: Yrast, 3 keV; Vib Es, 100 keV; B(E2)s, 10 Wu

Not all observables equally important; many multiply-test same physics

Including many yrast levels in a χ^2 test overweights that physics. The more, the worse it gets.

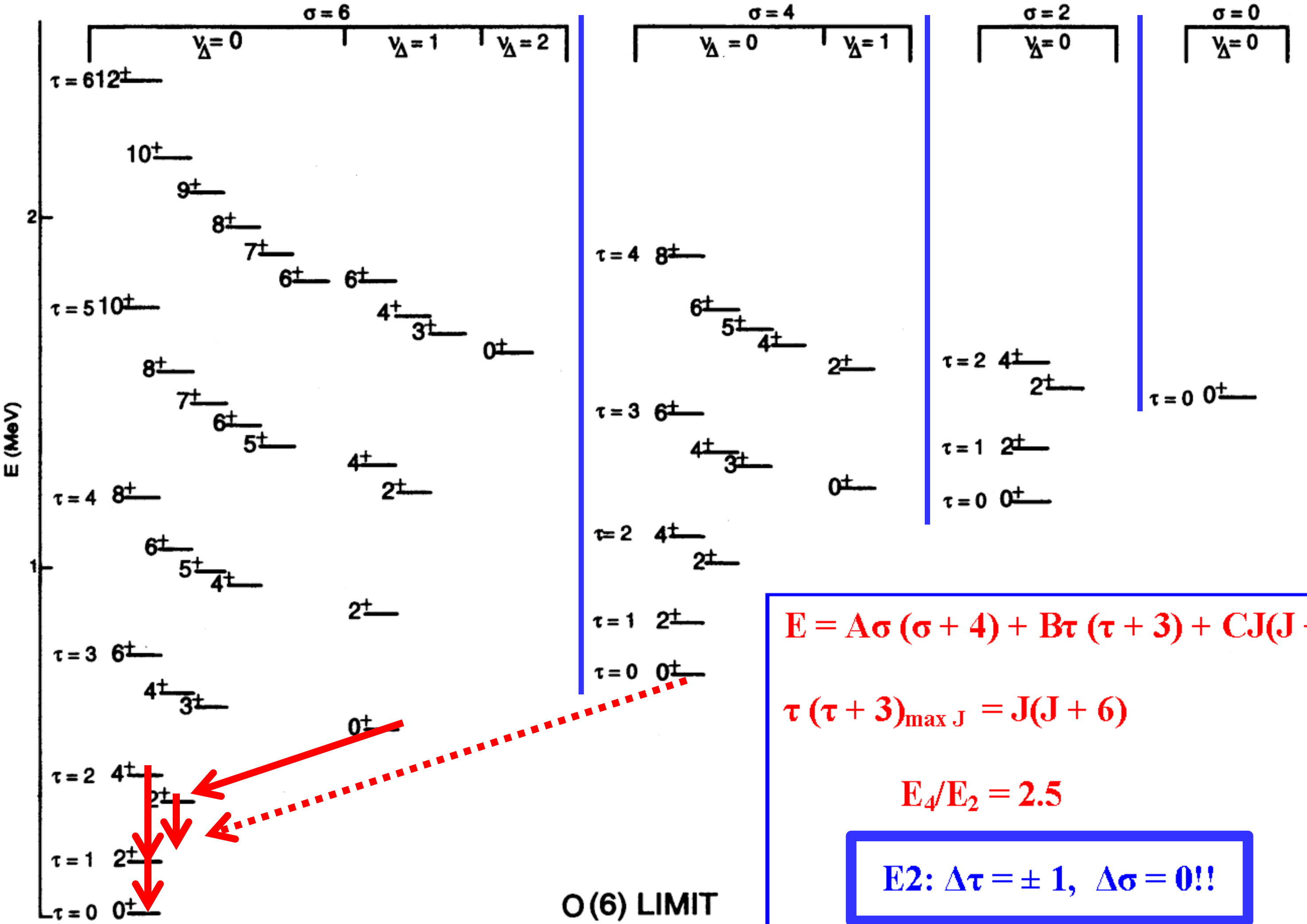
Vibrational bandhead energies

Bar

Rotational spacings

What are the key observables for testing collective models?

Choosing observables sensitive to specific physics



$$E = A\sigma(\sigma + 4) + B\tau(\tau + 3) + CJ(J + 1)$$

$$\tau(\tau + 3)_{\max J} = J(J + 6)$$

$$E_4/E_2 = 2.5$$

$$\text{E2: } \Delta\tau = \pm 1, \quad \Delta\sigma = 0!!$$

(σ,τ)

Parameters

Parameters

Dealing with multi-parameter models

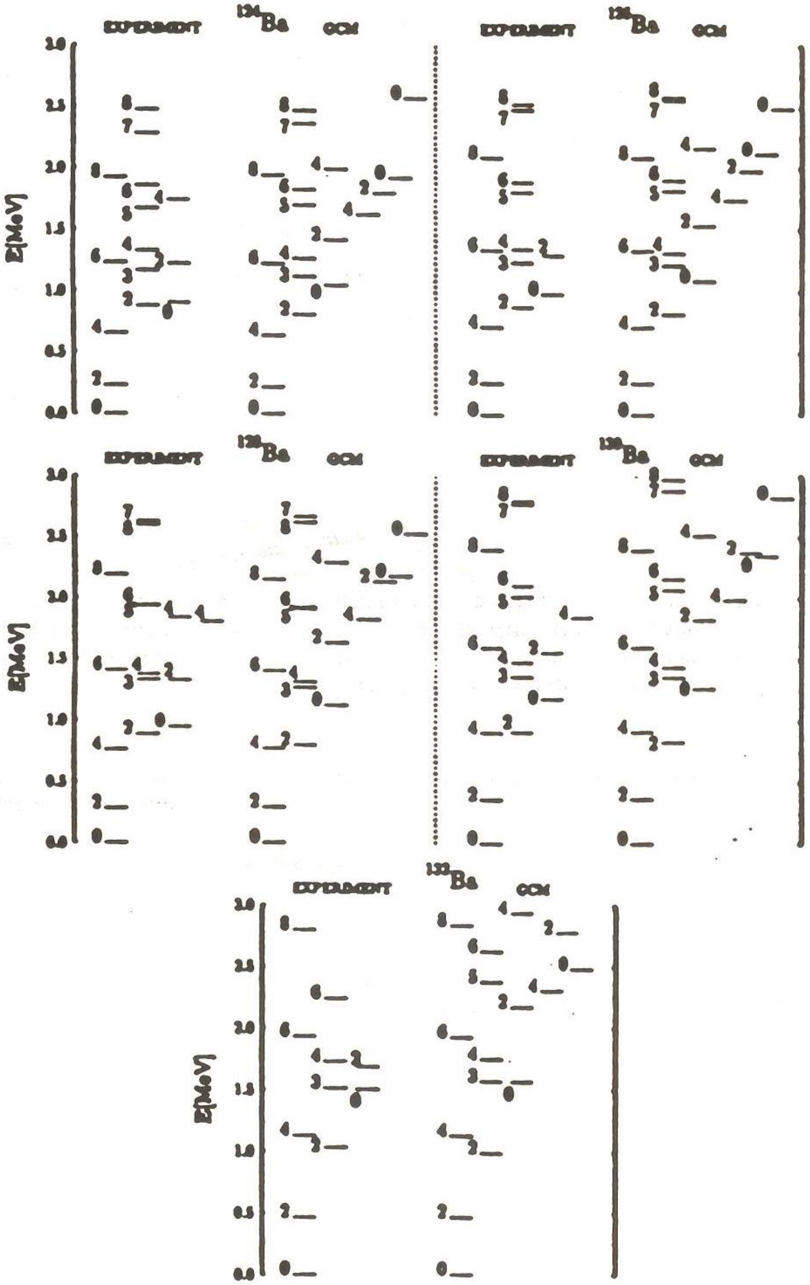


FIG. 3. Calculated and experimental level schemes of $^{124-132}$Ba.

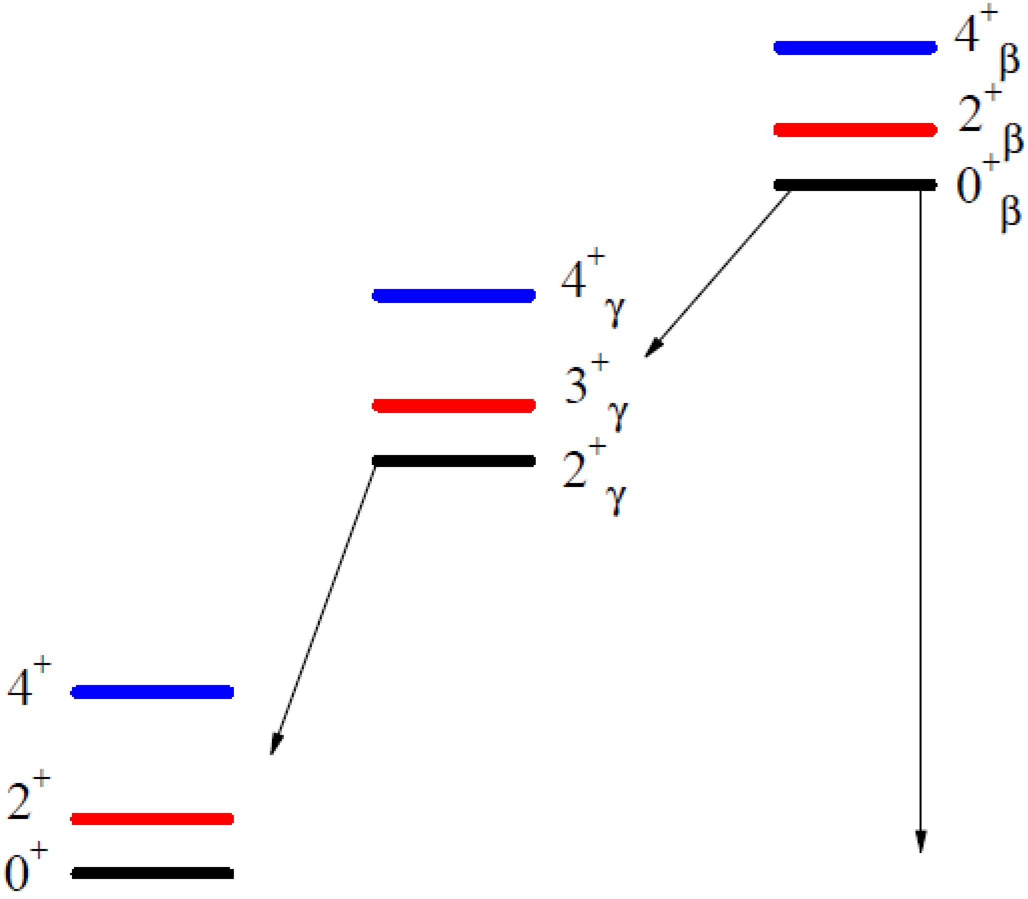
TABLE I. Parameters of the GCM Hamiltonian used in the present work. The only purpose of presenting their numerical values with a large number of significant digits is to ensure a reproducibility of the calculations. Some physical characteristics of the potentials are also displayed: the depth $V_{\min}$ and the position $\beta_{\min}$ of the absolute minimum ($\gamma_{\min} \approx 0$ in all cases considered), the PO difference $V_{PO}^{0^\circ-60^\circ} = \min[V(\beta,60^\circ)] - \min[V(\beta,0^\circ)]$ as well as the potential energy differences $V_{0^\circ-30^\circ} = \min[V(\beta,30^\circ)) - \min[V(\beta,0^\circ)]$ and $V_{30^\circ-60^\circ} = \min[V(\beta,60^\circ)] - \min[V(\beta,30^\circ)]$. The potential parameters, depths, and energy differences are given in MeV.

	^{124}Ba	^{126}Ba	^{128}Ba	^{130}Ba	^{132}Ba
B_2 (10^{-42} MeV s^2)	46.91602	53.8611	56.42193	62.70904	57.933
P_3 (10^{42} MeV^{-1} s^{-2})	-0.13	-0.118	-0.107141	-0.107602	-0.125873
C_2	-209.0632	-252.7933	-263.6945	-352.6598	-314.2383
C_3	135.8335	220.6479	248.7190	362.6218	442.1007
C_4	1708.726	3449.529	4323.475	8848.212	9517.914
C_5	-229.18361	-946.7563	-1371.759	-86.12527	8525.92
C_6	-36499.49	-50421.41	-41041.91	-15557.86	74370.15
D_6	36499.49	41910.09	32030.03	10191.77	-546.2191
$V_{\min}$	-5.7	-5.2	-4.8	-4.4	-3.5
$\beta_{\min}$	0.320	0.286	0.270	0.230	0.212
$V_{PO}^{0^\circ-60^\circ}$	1.7	1.8	1.6	1.6	1.7
$V_{0^\circ-30^\circ}$	2.0	1.7	1.4	1.0	1.0
$V_{30^\circ-60^\circ}$	-0.3	0.1	0.3	0.7	0.8

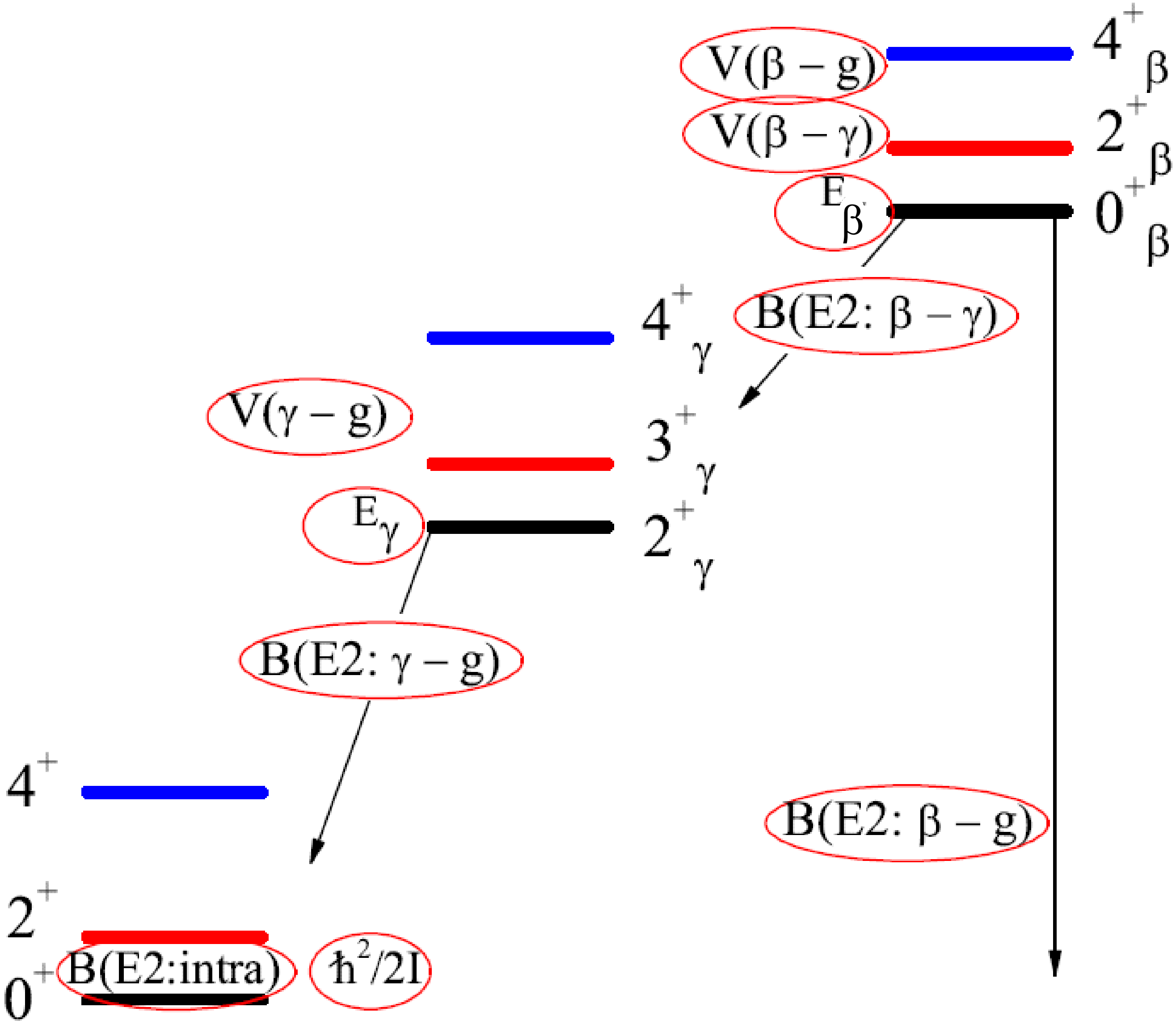
Parameters

Interpreting this level scheme with bandmixing

How many parameters?



Beware of parameters



Why do some models have so many and others so few parameters?

Compare above 10-15 parameter calculation with the IBA which obtains comparable or better fits with 2-3 parameters.

Why? It's the same physical system both are describing.
An answer sheds some light on the nature of models.

The IBA makes an ansatz: truncate shell model. That saves many parameters. But that ansatz is itself a kind of parameter choice – to set to zero the amplitudes of many shell model configurations.

One can thus often think of models as searches to select the appropriate degrees of freedom. Those choices are effectively physics-based parameterizations that don't appear as explicit parameters. The success or failure of those models teaches us about these ansatzes and the physics behind them

Summary

Beware of blind statistical optimizations

Always include theoretical uncertainties

Do not multiply fit the same physics

Choose observables that select specific physics

Be conscious of the number and nature of (often hidden) parameters.