Shape coexistence :

Introduction to theoretical shape coexistence studies

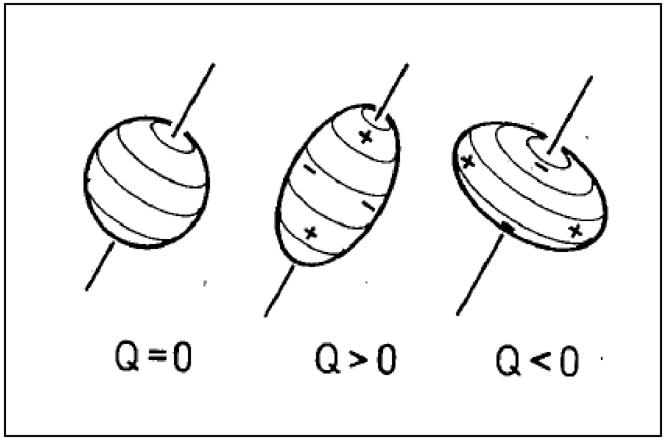
Kris Heyde
Department of Physics and Astronomy
University of Ghent

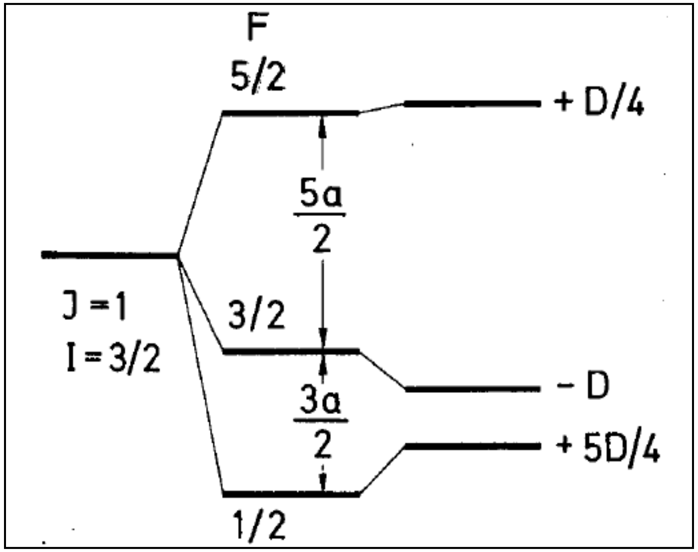
How to extract direct experimental information on nuclear shapes.

Earliest approach through studies of the interaction between electric moments (quadrupole,...) and the atomic electrons: study of the hyperfine structure of the optical spectra.

How to extract direct experimental information on nuclear shapes.

Interaction between electric moments (quadrupole,...) and the atomic electrons: study of the hyperfine structure of the optical spectra.





Magnetic dipole Electric quadrupole

Quadrupole deformation shows up as deviation from interval rule a.F

First hints of deformed nuclear shapes: a step back to the mid 30's

Schüler and Schmidt: Z. Phys. 94(1935),457: first experiment extracting a quadrupole deformed charge distribution ^{151,153}Eu

Casimir: Physica 7(1935),719 – theoretical description of the observed effect – proposal for quadrupole deformation

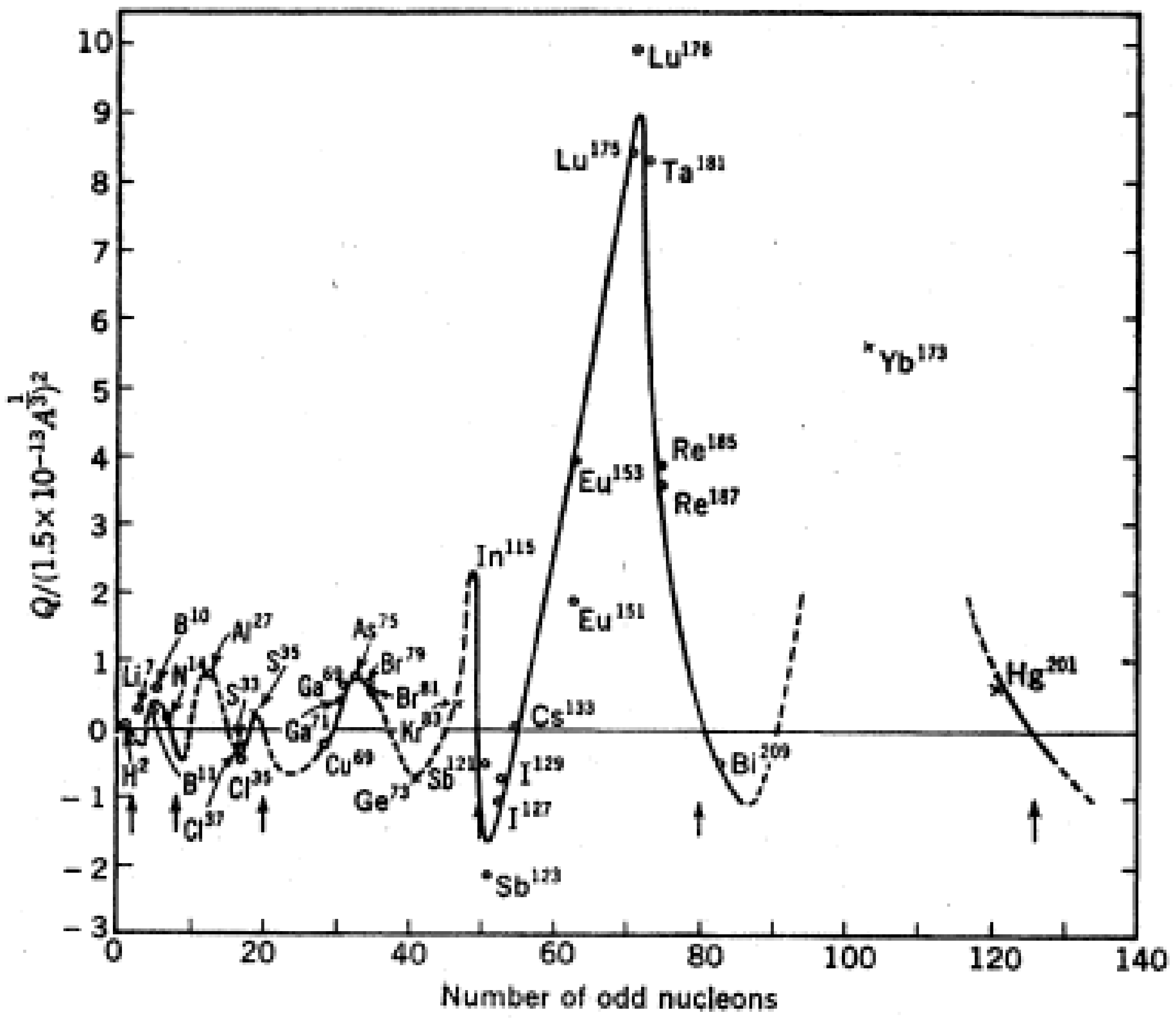
$$\Delta E_f = -e^2 \left\{ \frac{1}{r^3} \frac{3\cos^2\vartheta - 1}{(2j-1)j} \right\}_{j,j} \cdot \left\{ \frac{3z^2 - r^2}{(2i-1)i} \right\}_{i,i} \cdot \left[\tfrac{3}{8} C(C+1) - \tfrac{1}{2} i\, j\, (i+1)(j+1) \right]$$

mit

$$C = f(f+1) - i(i+1) - j(j+1).$$

Townes, Fowley and Low: Phys.Rev. 76(1949),1415 : systematics of nuclear quadrupole moments in odd-mass nuclei

Systematics as of 1949 data... opposed to s.p. picture



Quadrupole moments for odd-proton(circles) and odd-neutron (crosses) nuclei

High precision in study of nuclear moments (atomic physics)

Schüler and Schmidt (1935): anomalies in hyperfine structure – presence of a quadrupole component (Casimir (1936): proposes deformed shape)

Schmidt (1937): magnetic moments in nuclear ground states (and spins)

Townes, Fowley and Low (1949): nuclear quadrupole moment systematics

Time ready for major breakthroughs: clear-cut evidence for emerging concepts such as single-particle and collective motion in the atomic nucleus.

Maria Goeppert Mayer, J.Hans D. Jensen – 1963

"for their discoveries concerning nuclear shell studies"

On Closed Shells in Nuclei. II

MARIA GOEPPERT MAYER
Argonne National Laboratory and Department of Physics, University of Chicago, Chicago, Illinois
February 4, 1949

THE spins and magnetic moments of the even-odd nuclei have been used by Feenberg[1,2] and Nordheim[3] to determine the angular momentum of the eigenfunction of the odd particle. The tabulations given by them indicate that spin orbit coupling favors the state of higher total angular momentum. If strong spin-orbit coupling, increasing with angular momentum, is assumed, a level assignment different from either Feenberg or Nordheim is obtained. This assignment encounters a very few contradictions with experimental facts and requires no major crossing of the levels from those of a square well potential. The magic numbers 50, 82, and 126 occur at the place of the spin-orbit splitting of levels of high angular momentum.

Phys.Rev.75,1969 (1949)

On the "Magic Numbers" in Nuclear Structure

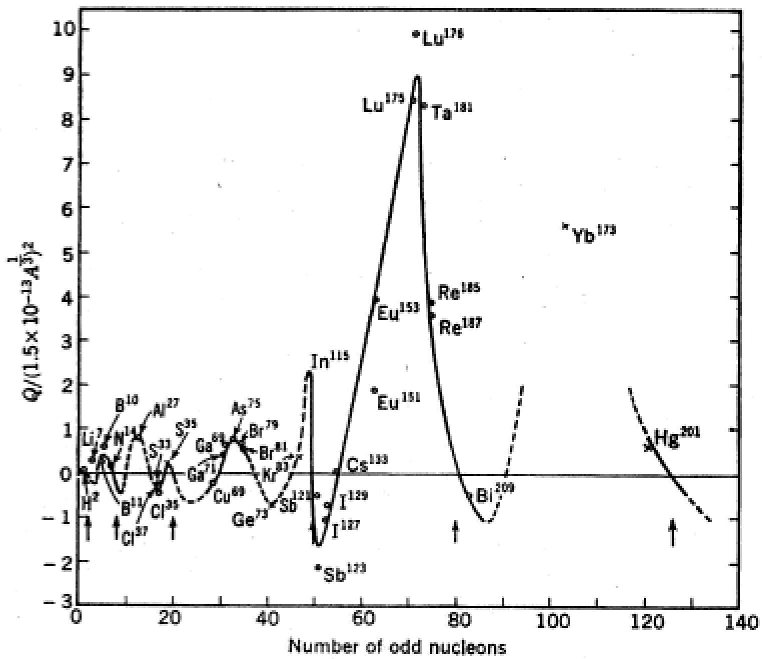
OTTO HAXEL
Max Planck Institut, Göttingen
J. HANS D. JENSEN
Institut f. theor. Physik, Heidelberg
AND
HANS E. SUESS
Inst. f. phys. Chemie, Hamburg
April 18, 1949

A SIMPLE explanation of the "magic numbers" 14, 28, 50, 82, 126 follows at once from the oscillator model of the nucleus,[1] if one assumes that the spin-orbit coupling in the Yukawa field theory of nuclear forces leads to a strong splitting of a term with angular momentum l into two distinct terms $j=l\pm\frac{1}{2}$.

Phys.Rev.75,1766(1949)

Aage Bohr, Ben Mottelson and James Rainwater – 1975

“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”



More hints of deformation came through clever experimenting combined with parts of serendipity

- Early "Coulomb excitation" and work carried out by Day, Huus at Caltech (1952) and McClelland and Goodman (1953) at MIT

  Clear indications of rotational band in Ta nuclei

- Study of alpha decay in the actinides showed first excited states that only could be explained through a collective type of excitation of the whole nucleus. (Asaro and Perlman , PR 92 (1953) 694
  as the result of discussions between A. Bohr and the group at LBL
  (priv. comm. to J.L.Wood from John Rasmussen)

Conflicting situation in the early 50's: how to reconcile?

MICROSCOPIC

Single-particle modes of motion:
Nuclear shell model
explaining many experimental data
(μ, J, stability and shell-structure)

MACROSCOPIC

Deformed nuclear shape:
Dynamics of collective liquid drop model
explaining rotational bands (o-o, o-e) in
Coulomb excitation

Conflicting situation in the early 50's: how to reconcile?

MICROSCOPIC

Single-particle modes of motion:
Nuclear shell model
explaining many experimental data
(μ, J, stability and shell-structure)

MACROSCOPIC

Deformed nuclear shape:
Dynamics of collective liquid drop model
explaining rotational bands (o-o, o-e) in
Coulomb excitation

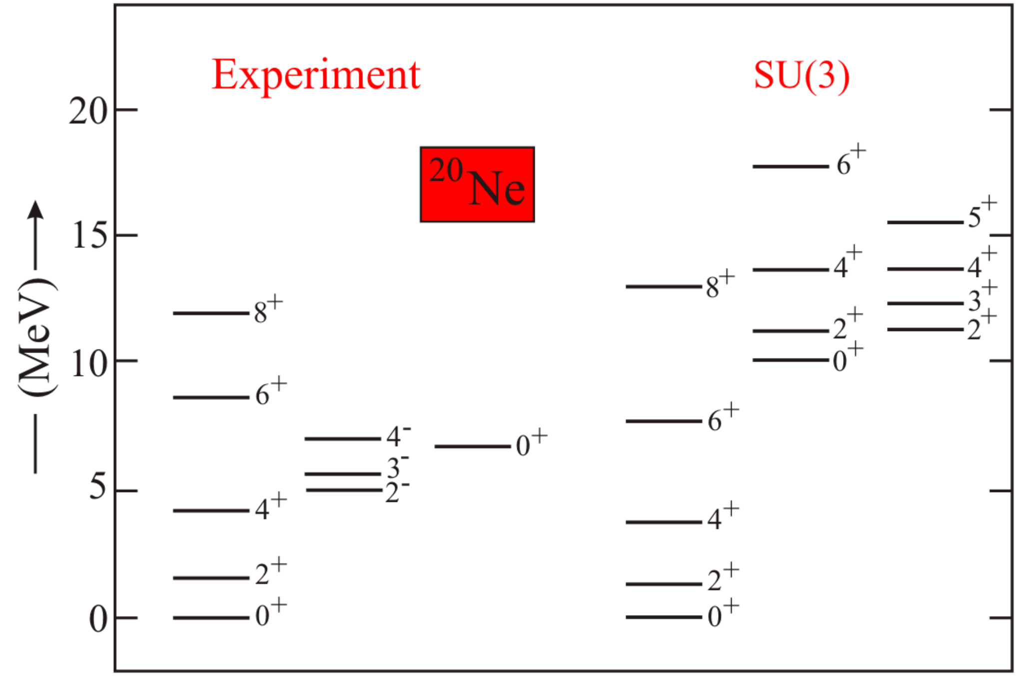
Indications that the two sides were more closely connected then orginally thought.

Nilsson model shifting attention from a deformed density to a deformed single-particle potential (Nilsson 1955)

A few years later, appearance of the power of symmetries in describing nuclear structure degrees of freedom: J. P.Elliott (1958)

Elliott's SU(3) model (1958) : exact solution to a simpified model

$$H=\sum_{k=1}^{A}\left[\frac{p_k^2}{2m}+\frac{1}{2}m\omega^2 r_k^2\right]-\chi Q\cdot Q$$



Rotational relation J(J+1)

Deep link between spherical shell-model (mixing of spherical orbitals) and concept of intrinsic state, specific for mean-field approach and rotational structures

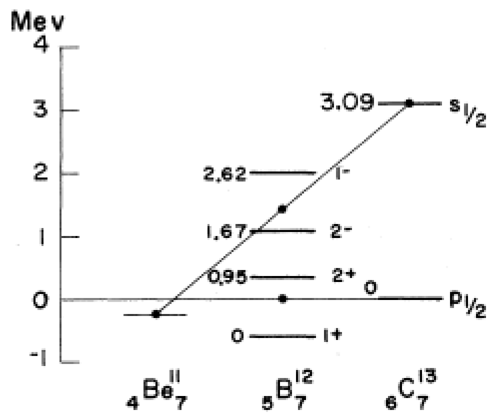
Early anomalies in the shell-model standard ordering

R F Christy and W A Fowler, Phys. Rev.96, 851(A) 1954

VOLUME 4, NUMBER 9 PHYSICAL REVIEW LETTERS MAY 1, 1960

ORDER OF LEVELS IN THE SHELL MODEL AND SPIN OF Be^{11}*

I. Talmi and I. Unna
Department of Physics, The Weizmann Institute of Science, Rehovoth, Israel
(Received April 4, 1960)



Early use of monopole energy shift

$$\langle j^2(J=0)j'|V_{1n}+V_{2n}|j^2(J=0)j'\rangle$$

$$=2\sum_{J=|j-j'|}^{J=j+j'}(2J+1)\langle jj'J|V|jj'J\rangle \Big/ \sum_{J=|j-j'|}^{J=j+j'}(2J+1). \quad (1)$$

R F Christy and W A Fowler, Phys. Rev.96, 851(A) 1954

Nature of the ½- excited state in 19F : proposal as a
p-hole 4 sd- particle configurations , explaining similar
½- states in 17O (3.07 MeV) and in 17F 3.10 MeV) as
the addition of 4 sd particles to 13C and 13N, respectively.

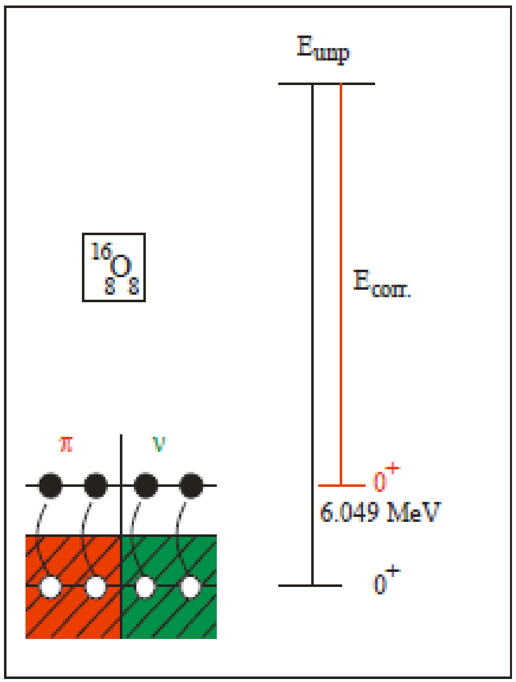
Early hints for strongly correlated excited states

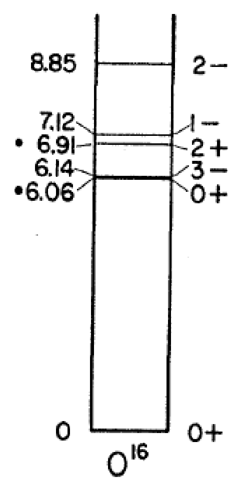
PHYSICAL REVIEW VOLUME 101, NUMBER 1 JANUARY 1, 1956

Interpretation of Some of the Excited States of 4*n* Self-Conjugate Nuclei*

H. MORINAGA†
Department of Physics, Purdue University, Lafayette, Indiana

(Received August 5, 1955)



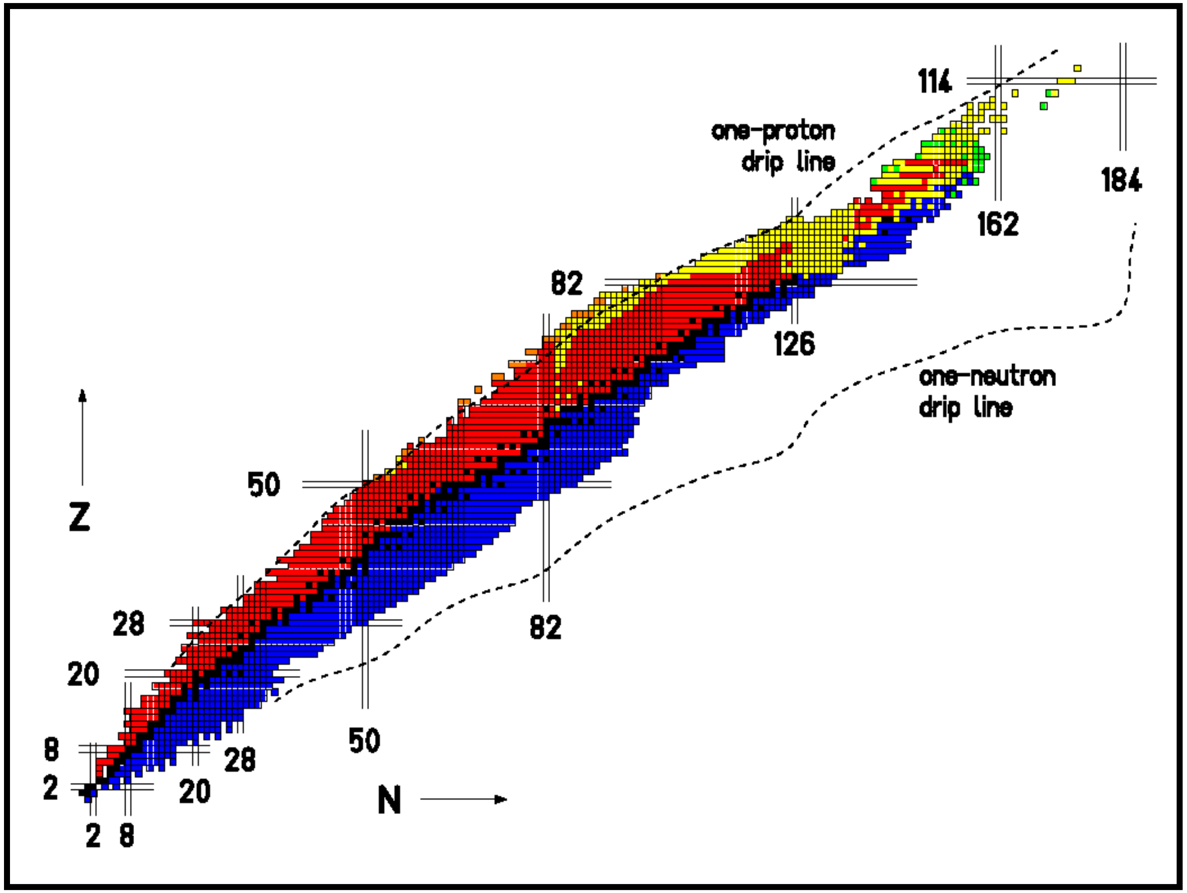


G.E. Brown, INPC, Paris (1964),129
G.E. Brown and A.M.Green, NP85(1966),87

1. INTRODUCTION

THE energy level structures of 4*n*-type light nuclei, like Be^8, C^{12}, O^{16}, Ne^{20}, and Mg^{24}, show some characteristic features which are not quite easy to explain from simple shell-model theories. The alpha-particle model[1] has been considered as a hopeful alternative for describing these levels, and recent re-examination of the alpha-particle model of the O^{16} nucleus[2] seem to show a remarkable agreement with experiment.[3] However, there are still several difficulties with this model, especially in assigning the first dilatational vibration to the 6.06-Mev, 0^+ pair-emitting level.[1,2,4]

Recently Christy and Fowler proposed a "hole configuration," or a configuration where four *p* particles are raised up to the next shell (*s*, *d* orbits) for explaining this state, in analogy to the low-lying $\frac{1}{2}-$ state in F^{19} and the $\frac{1}{2}-$ state at around 3-Mev excitation of O^{17} and F^{17}.[5] Schiff also investigated a two-nucleon excitation for the same state,[6] and concluded that in order to account for the observed lifetime of this state a model which is more collective than the independent-particle model with pair interaction and less collective than the conventional alpha-particle model is necessary. Since, however, such 0^+ states have been found in all 4*n* self-conjugate nuclei up to Ne^{20} at around the same energy, it is desirable to try to find a more general argument in connection with other level characterictics. It is the purpose of this note to suggest a possible interpretation of these 0^+ states as rotationless states of strongly deformed configurations.

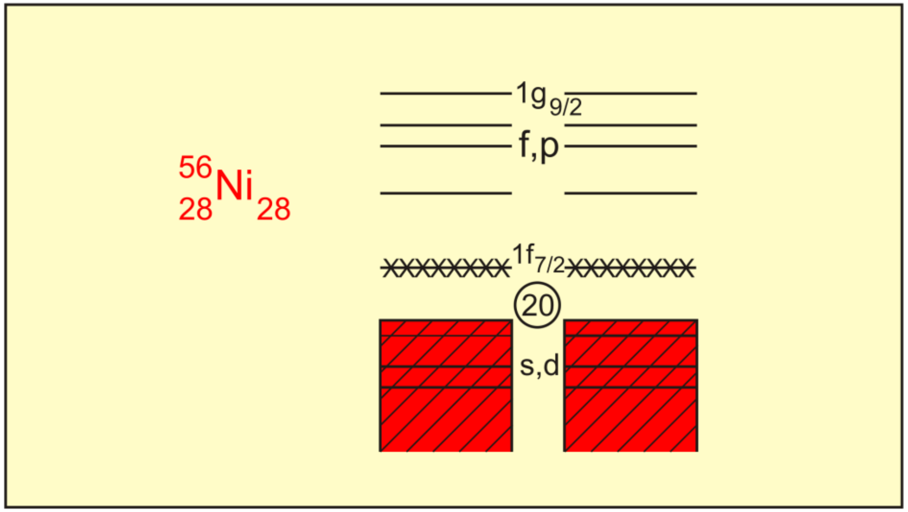


Aim : explore conditions in the nuclear landscape for coexistence of various phases.

Importance of the interplay between stabilizing effect of spherical closed shells versus the residual interation energy for certain distributions of valence protons and neutrons or excitations across 'closed' shells

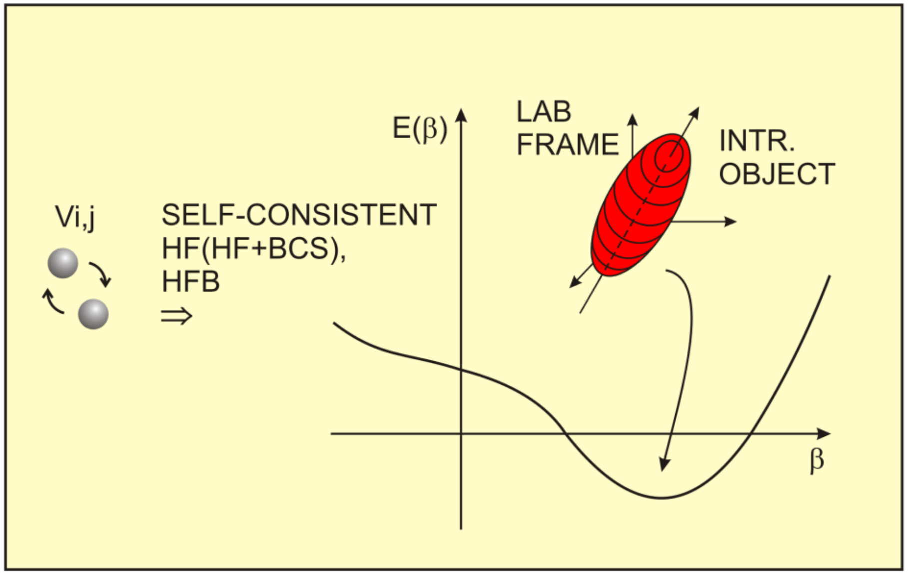
SHAPE COEXISTENCE: SHELL-MODEL AND MEAN-FIELD APPROACH

A. Use spherical shell model:
closed shells plus residual
interaction binding energy



B. Nucleons interacting through
V(i,j) n-n force generate
mean-fields.

Self-consistent calculations
imply deformed mean fields
in many cases



Importance of symmetries: quadrupole SU(3), Bohr-Mottelson Collective model, IBM,...

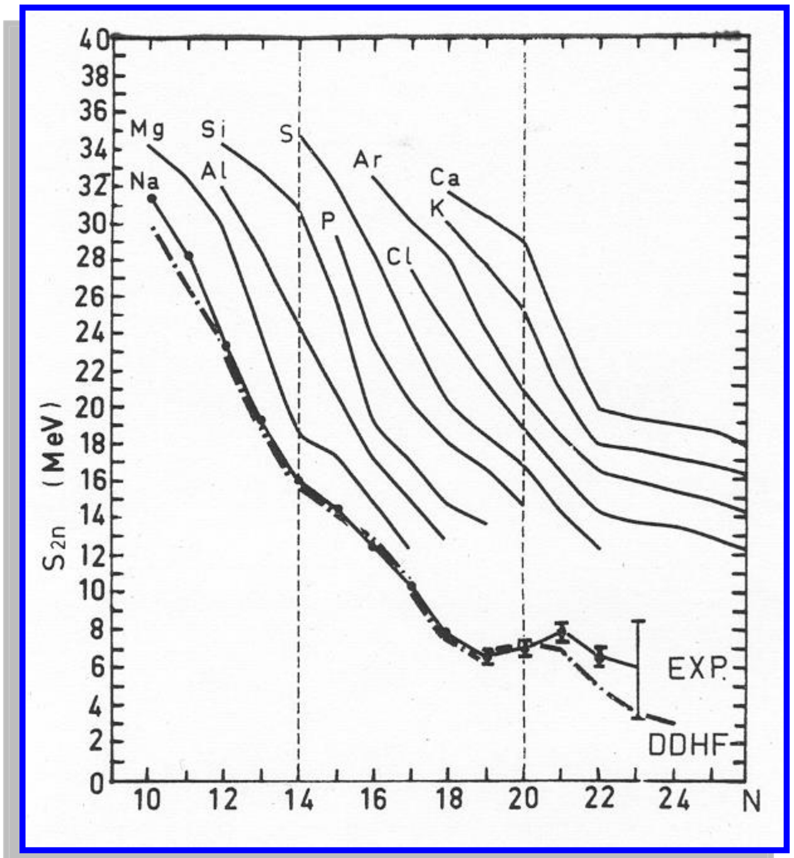
Nuclear shell-model

Mean-field methods

Symmetries in nuclei

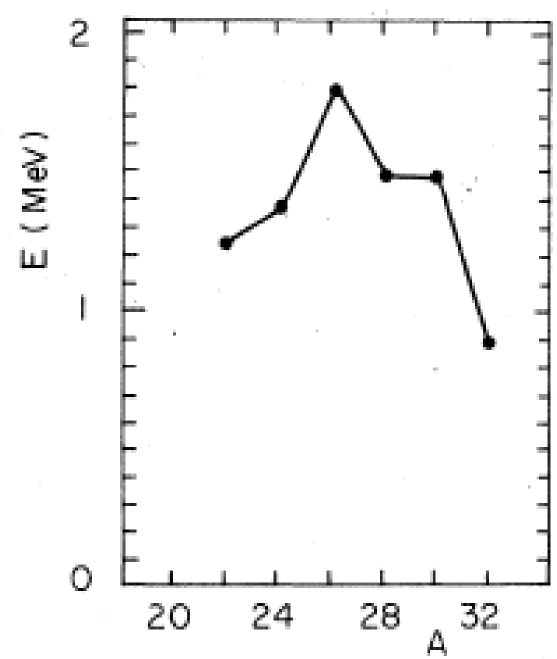
A. SPHERICAL SHELL-MODEL

Exploring the N=20 region (neutron closed-shell)
.... with unexpected results.



Thibault et al. PRC12(1975)

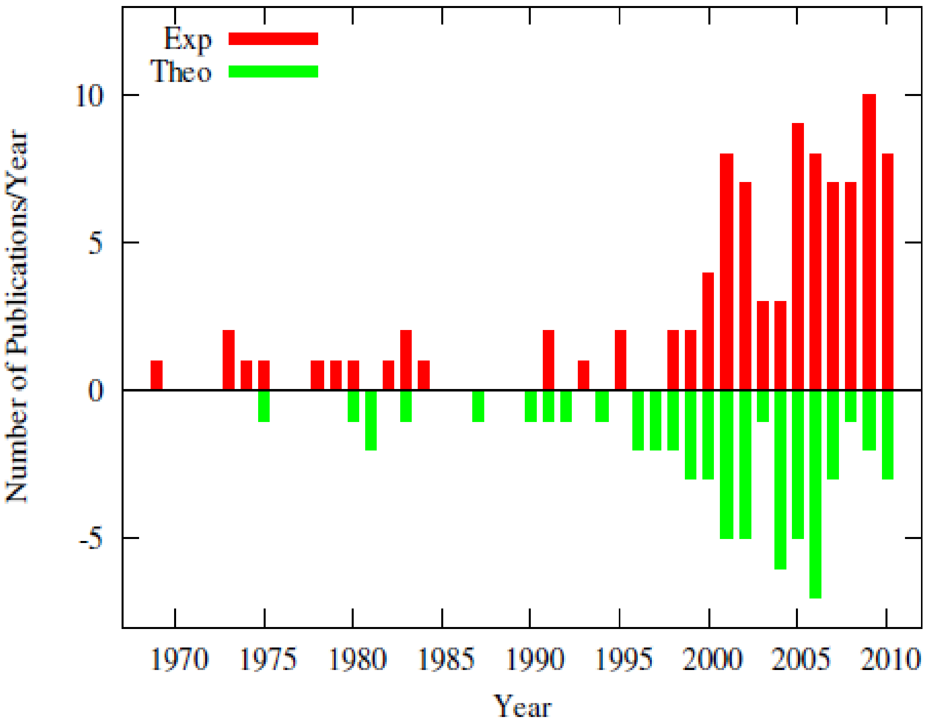
2^+_1 excitation energy (β-decay)



Détraz et al.,
PRC 19 (1979)

N=20 region

"Collapse of the conventional shell-model ordering in the very-neutron-rich isotopes of Na and Mg", B.Wildenthal and W.Chung, PRC22(1980)

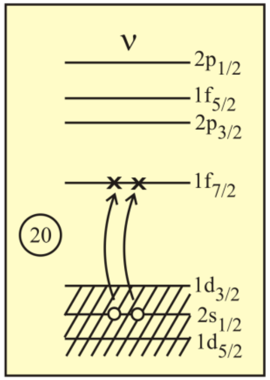


H.Scheit, J.Phys:conf.series 312(2011)

Detailed spectroscopic studies

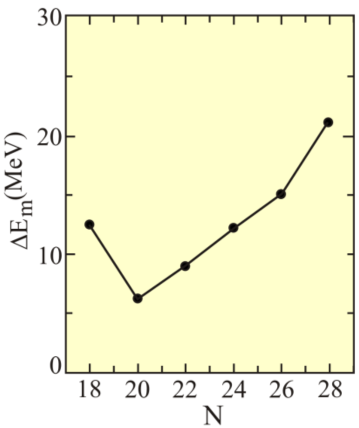
It took about 4 decades to construct the complete experimental picture.

N=20 shell gap

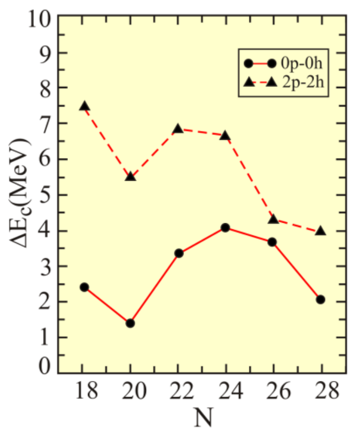


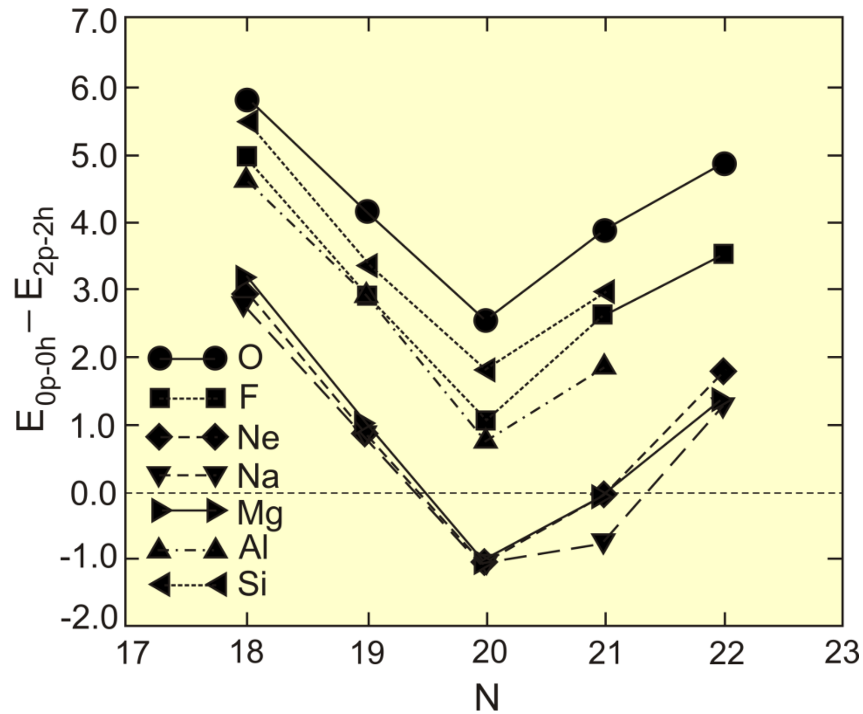
Mg NUCLEI

MONOPOLE GAP FOR
N= 20 2p-2h
CONFIGURATION



CORRELATION ENERGY

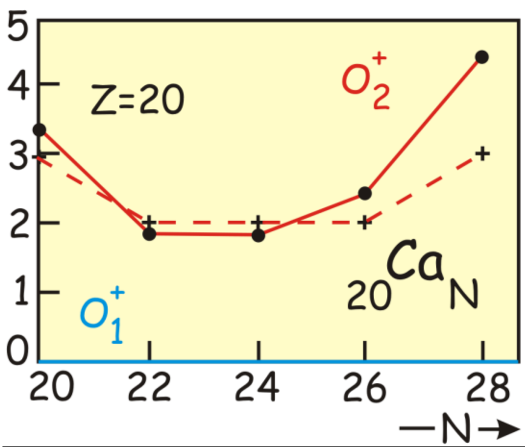


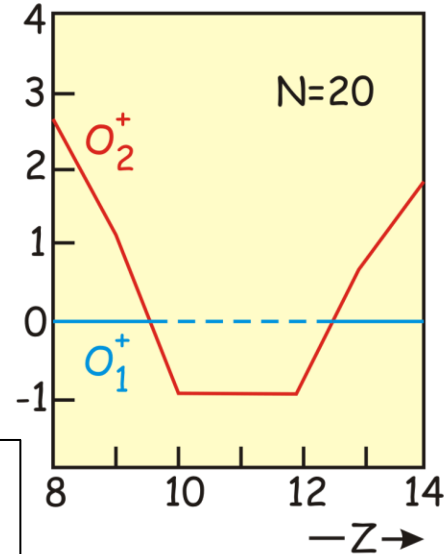


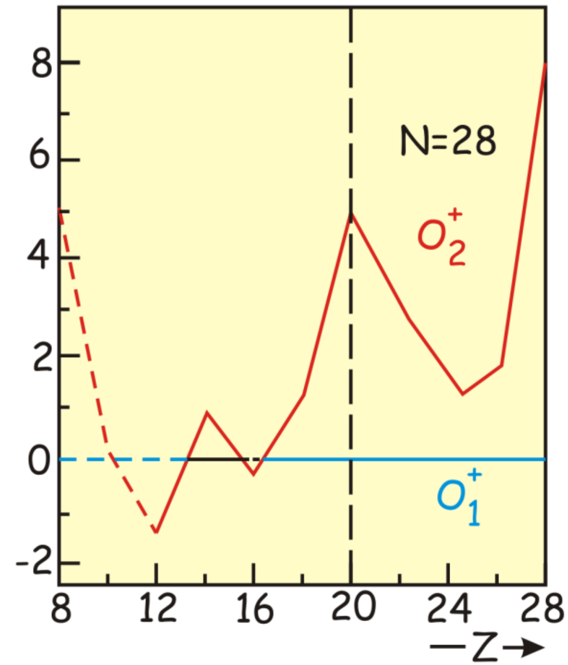
E. Caurier et al., PRC58 (1998), 2033

Inversion of spherical and
deformed configurations
→ region of shape coexistence.

Shell-model studies at Z, N=20; Z, N=28,...





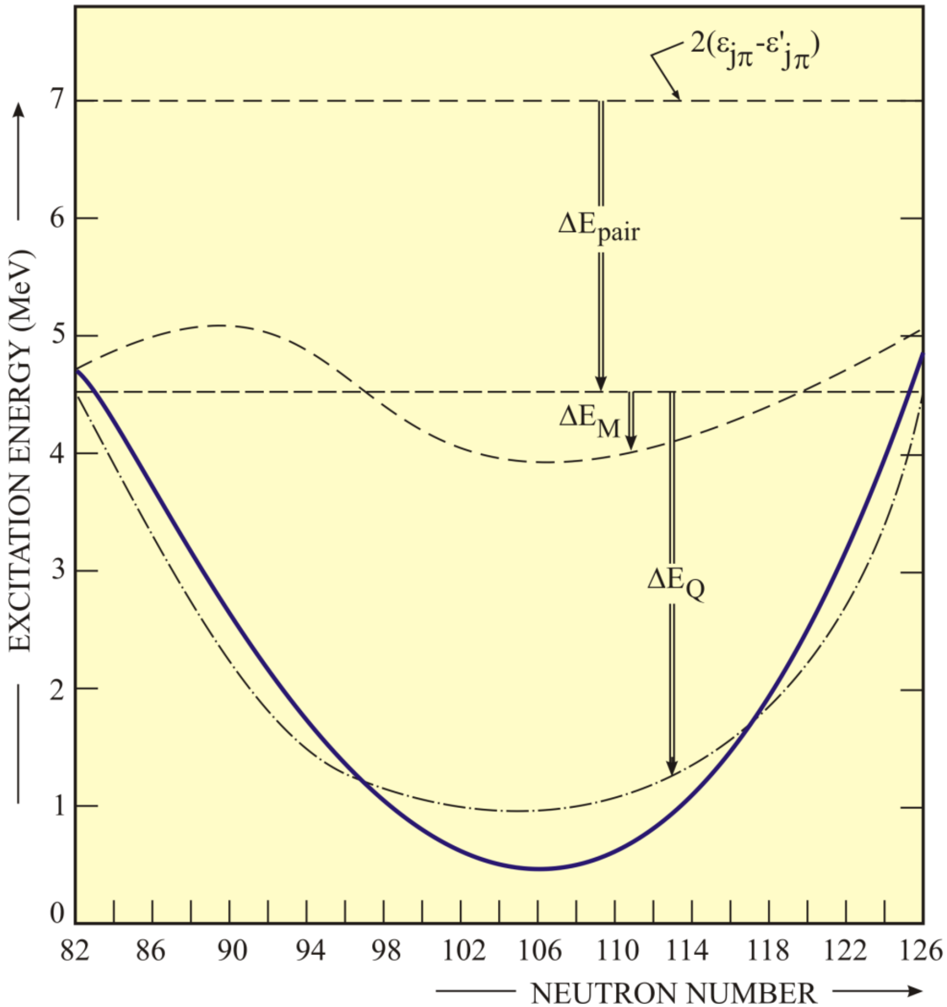


Caurier, Martinez-Pinedo, Nowacki, Poves, Zuker SM papers

- Competition between <u>monopole field</u> (energy needed to create np-nh excitations) and <u>"correlation" energy</u> (spherical-deformation)

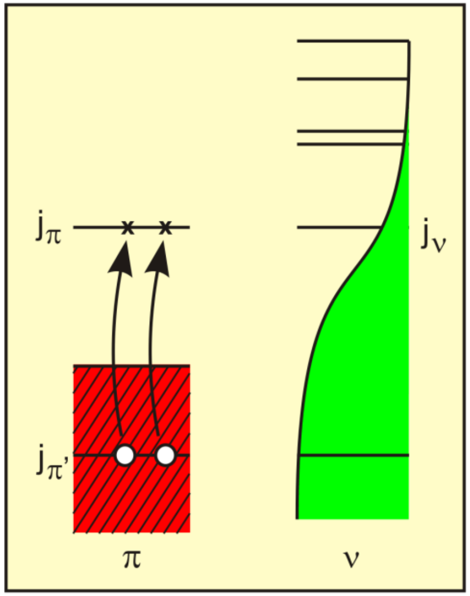
- Correlation energy $\propto$ <u>number</u> of valence nucleons $n_{val.}$ times <u>number</u> of excited pairs Δn_{p-h}.
  Property of quadrupole force.

Huge model space cannot be extended, including p-h excitations $\Rightarrow$ symmetry as guide to truncation.



Consider lowest 2p-2h excitations across closed shells.

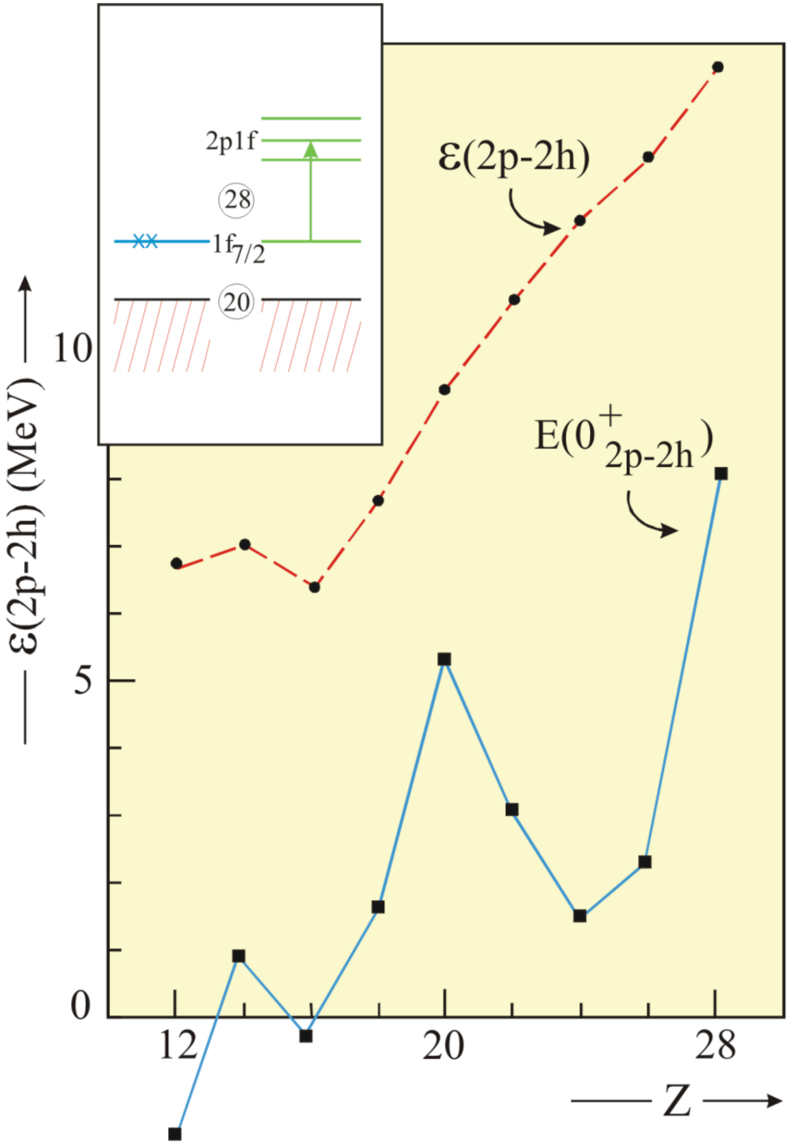
$Q_\pi.Q_\nu$ quadrupole-quadrupole force

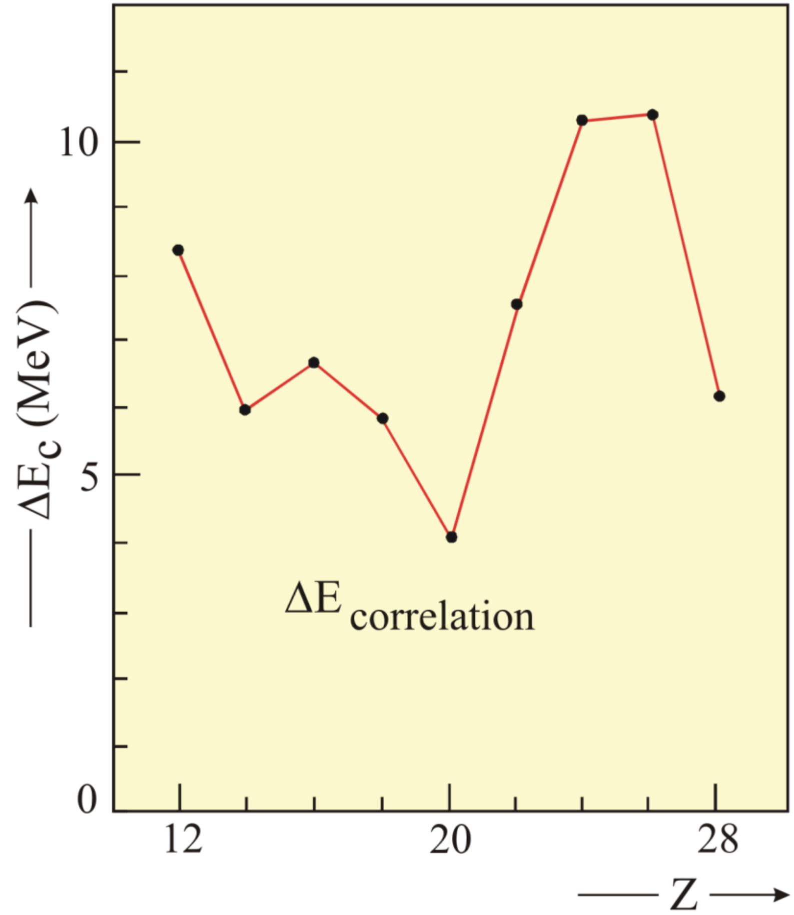


$$E_{intr.}(0^+) \simeq 2(\varepsilon_p - \varepsilon_h) + \Delta E_{pair.} + \Delta E_{mon.} + \Delta E_{quad.}$$

$$\Delta E_{quad.} \simeq 2\kappa N_\nu . \Delta N_\pi$$

N = 28 GAP

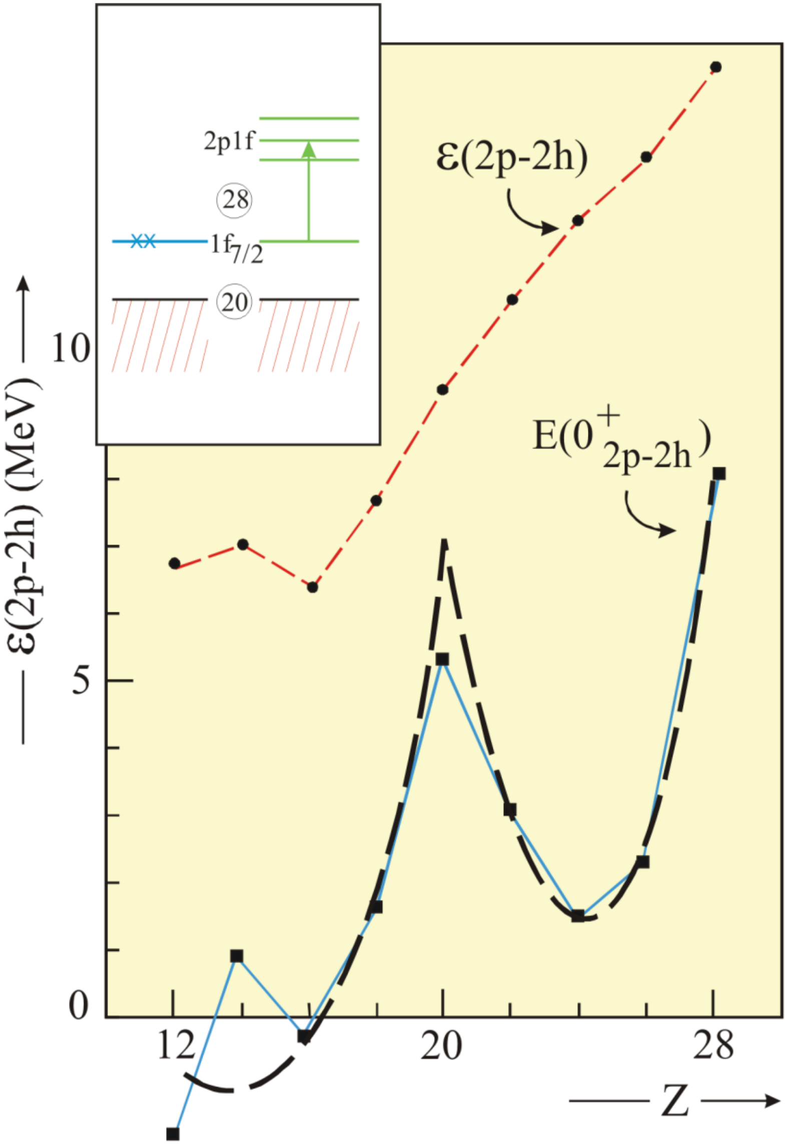


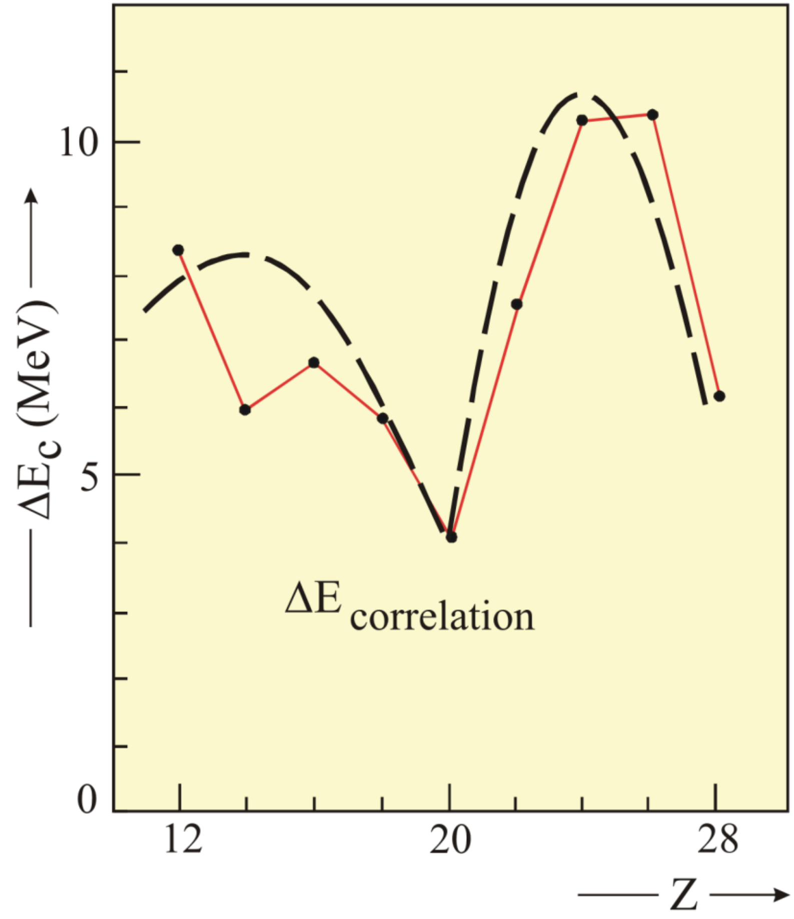


E. Caurier et al., NPA742(2004), 14

$E(0^+_{2p-2h}) = \varepsilon(2p\text{-}2h) - \Delta E_{correlation}$

N = 28 GAP

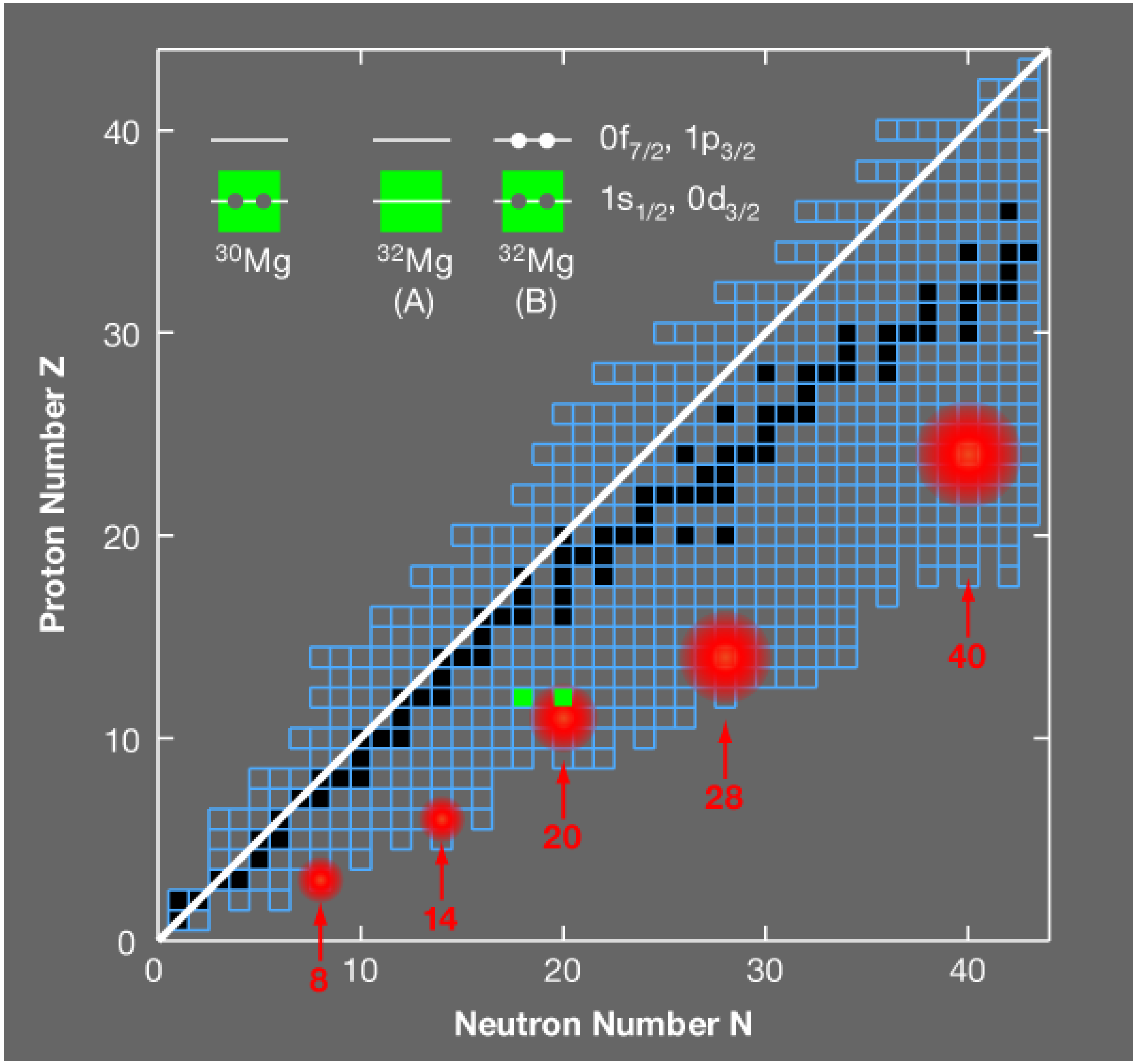




E. Caurier et al., NPA742(2004), 14

$E(0^{+}_{2p-2h}) = \varepsilon(2p\text{-}2h) - \Delta E_{correlation}$

B. A. Brown – Viewpoint Physics 3, 104 (2010)



See talk of Alfredo Poves for extensions and connnections

The spherical shell model basis for shell-model calculations is based on a formulation in the lab system. Deformation indirect through extensive comparions of calculated observables with the data.

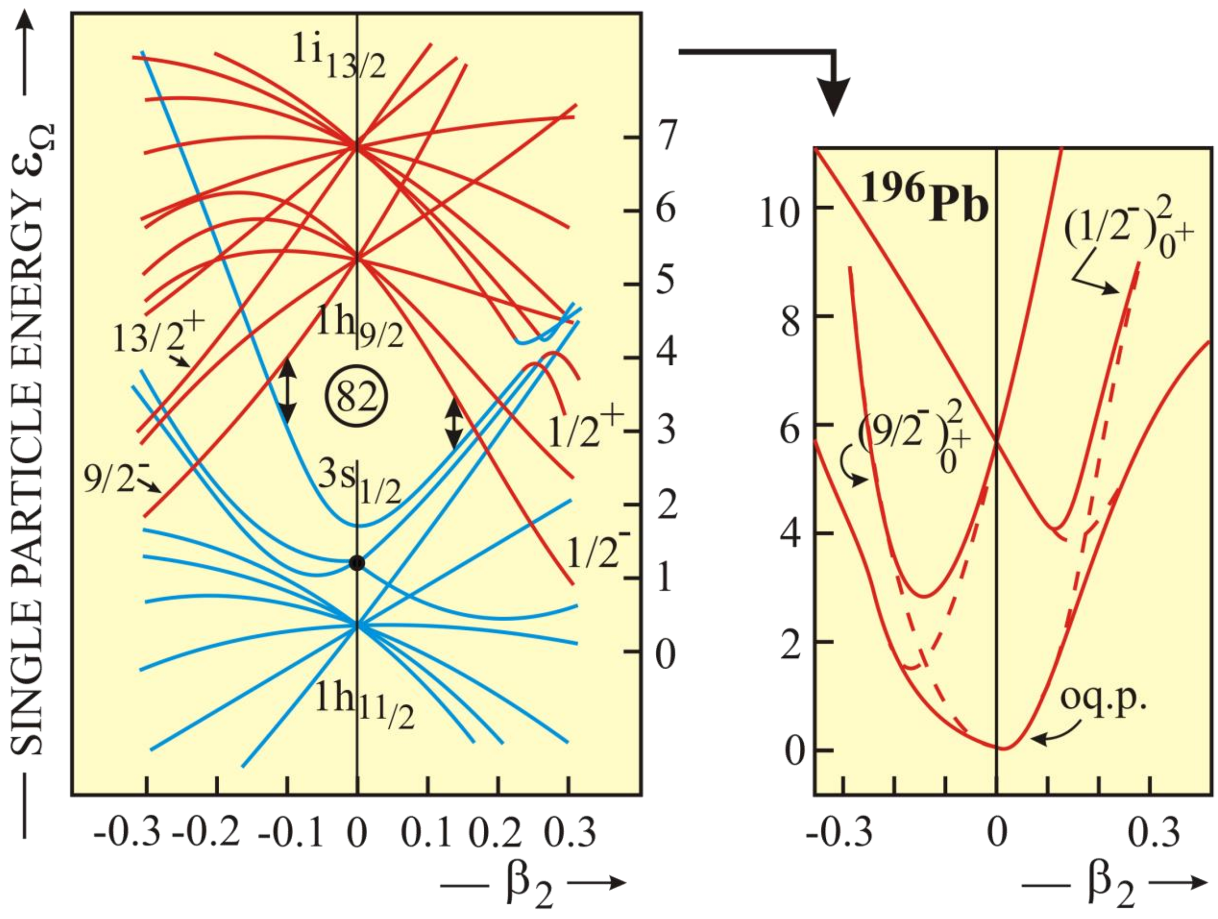
Elliott has indicated in 1958 an intimate connection between the lab system formulation and deformation using the fact that the spherical harmonic oscillator basis has an underlying SU(3) symmetry and was using a Q.Q interaction to solve the eigenvalue problem exactly (for the sd shell).

Incorporating extension of the Elliott model towards quasi-SU(3) (Zuker et al. , 1995) and pseudo-SU(3) (Arima et al., 1969 and Hecht and Adler, 1969), the shell-model could be truncated allowing to treat very large model spaces.

(see talk of Alfredo Poves)

B. APPROACH : NATURAL DESCRIPTION VIA DEFORMED MEAN - FIELD

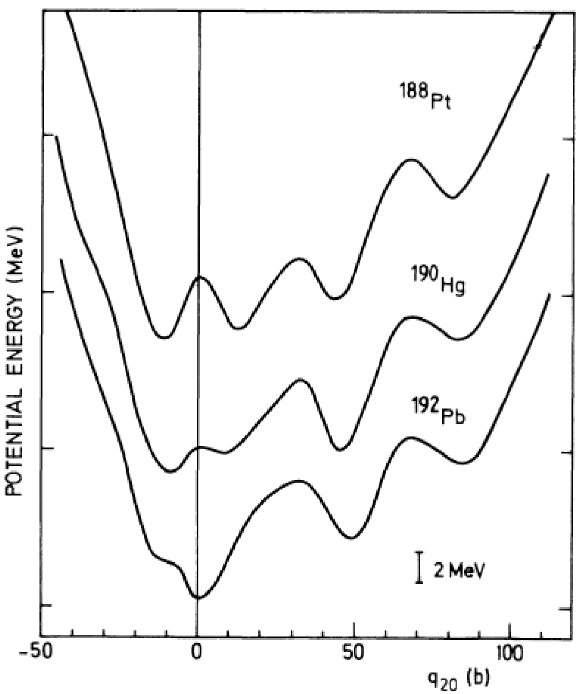
(Nilsson, Deformed WS,HF(B)..)



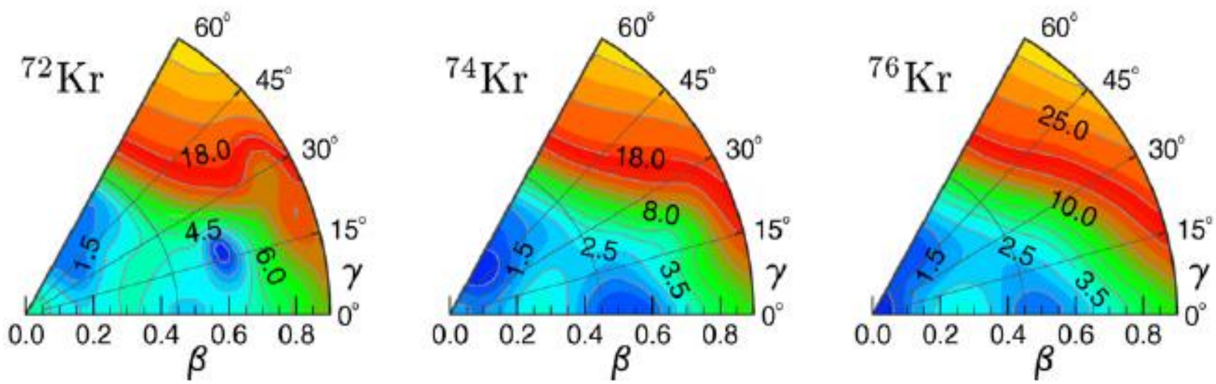
- LIQUID DROP +[SHELL+PAIRING CORR.]
- DEFORMED HFB

Comparing advances in constrained HFB calculations: two decades

Gogny D1S force



$$V(q) = \langle \Phi_q | H | \Phi_q \rangle - E_{ZP}(q)$$



Girod et al., PRL62(1989)

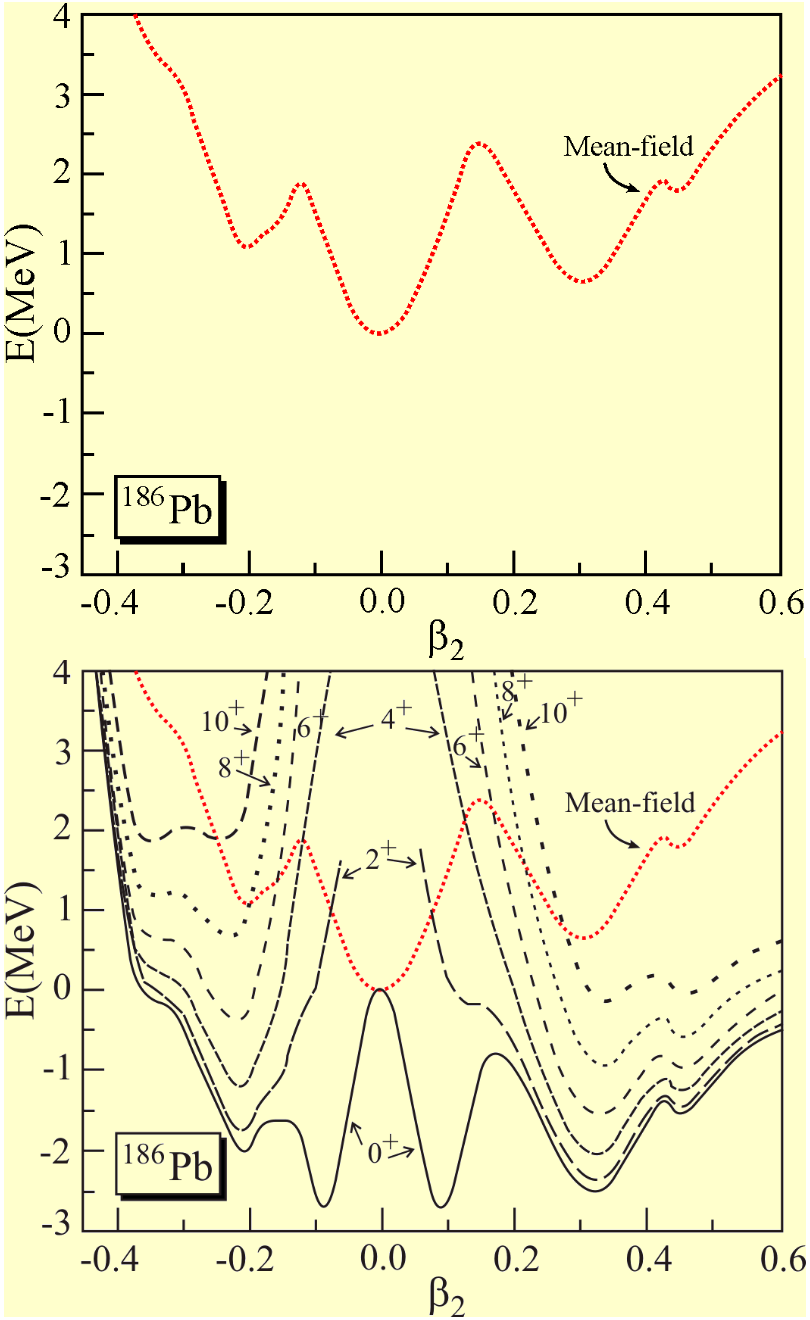
Girod et al., PLB676(2009)

Only the static part : potential energy

Intrinsic state - Mean-field energy
E(Z,N,q)

Restoration of broken symmetries:
angular momentum projection - E(Z,N,J,q)

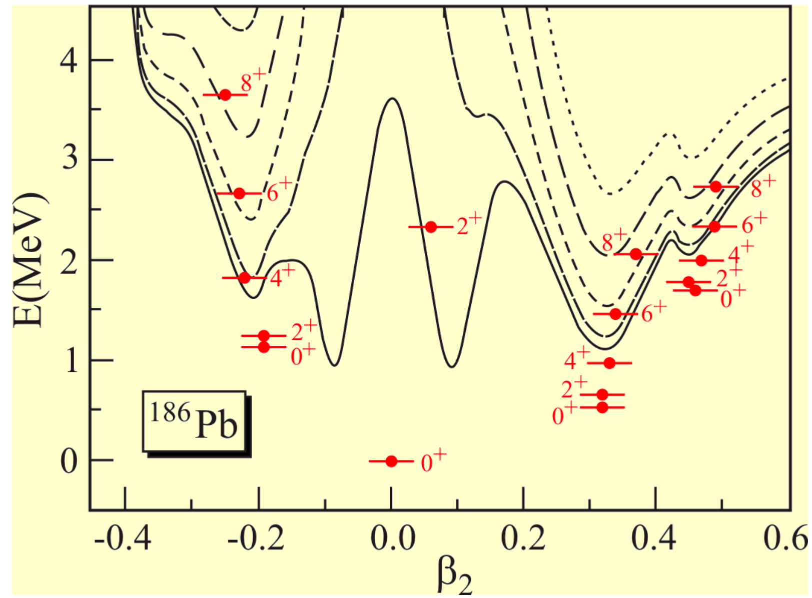
APPLICATION TO THE Pb nuclei
Duguet et al., Phys.Lett. B559(2003)



Need to go beyond mean field: seminal papers of Hill and Wheeler (1953), Griffin and Wheeler (1957).

GCM: variational methods now considering a continuous collective variables.

⇒ collective dynamics



Duguet et al., Phys.Lett. B559(2003)

See talks of M.Bender, T. Niksic and T.R. Rodriguez for most recent results

MERGING MEAN–FIELD WITH SHELL-MODEL METHODS?

Spherical shell model

Limited to start of the sdg shell model space using spherical h.o. potential.

Multi-p multi-h excitations give rise to configurations with increasing collective behavior (see ^{40}Ca).

Truncation using symmetries

Deformed mean field

Static part is only a first guide.
Need for dynamics.

Mixing of many projected |J,M,q> states to construct collective wave functions and energies

GOA approximation allows to extract collective Hamiltonian (BM type).

Try to combine the best of both methods

Optimizing the basis through Monte-Carlo methods of the model space, which operates as an “importance sampling” of the entire many body space (Otsuka 2001) aims at constructing deformed Slater determinant wave functions that are angular momentum and parity projected.

The approach called Monte-Carlo Shell Model (MCSM) allows to extract the intrinsic deformation characteristics by calculating the overlap between the wave function and the projected deformed Slater determinant basis wave functions and evaluating the corresponding quadrupole moments Q_0 and Q_2 (Tsunoda plots or T-plots).

(see talk of Taka Otsuka)

Symmetries
Algebraic approaches

SYMMETRY CONCEPTS IN NUCLEAR STRUCTURE

The early steps

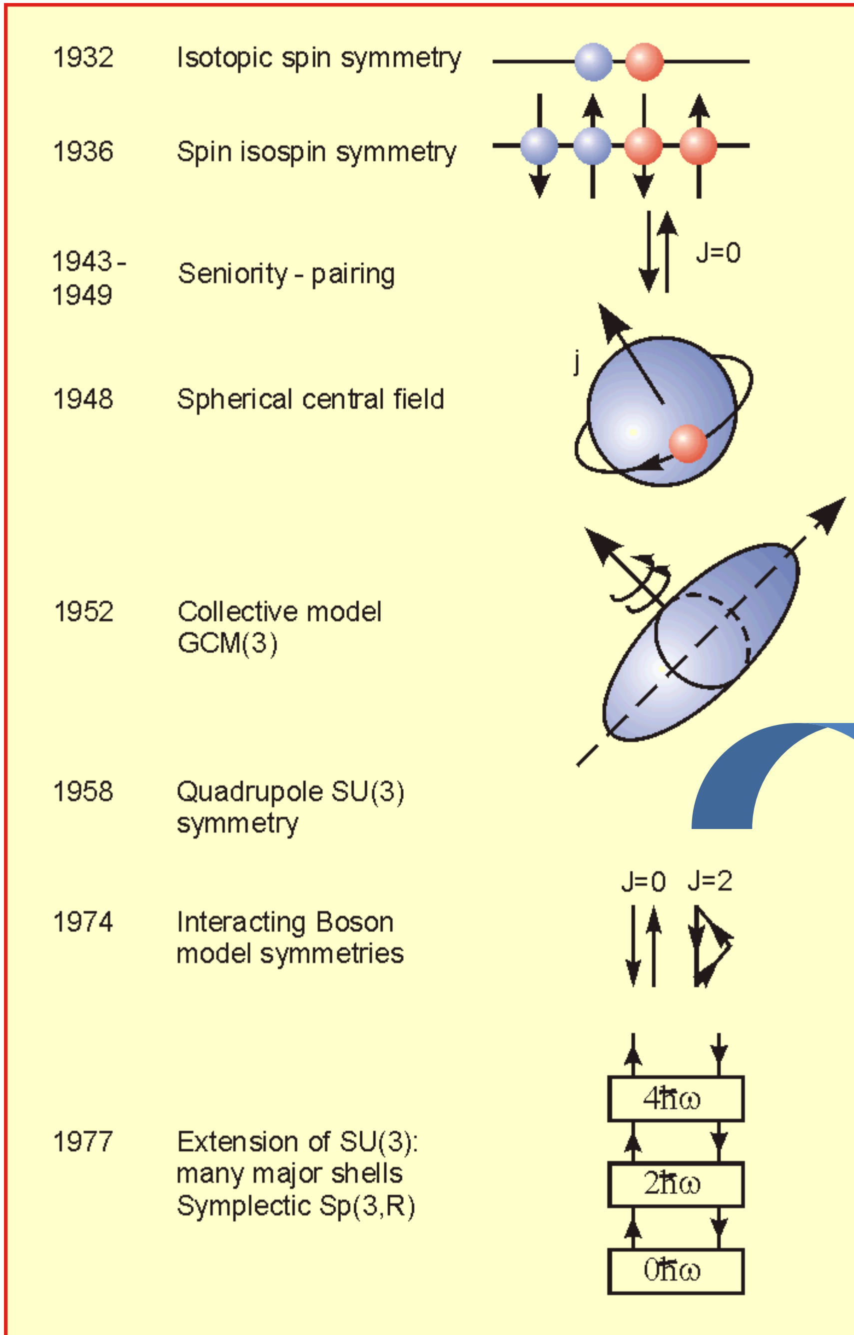
W. Heisenberg
Z.Phys.77(1932)

E.P. Wigner
Phys.Rev.51(1937)

G. Racah
Phys.Rev.76(1949)

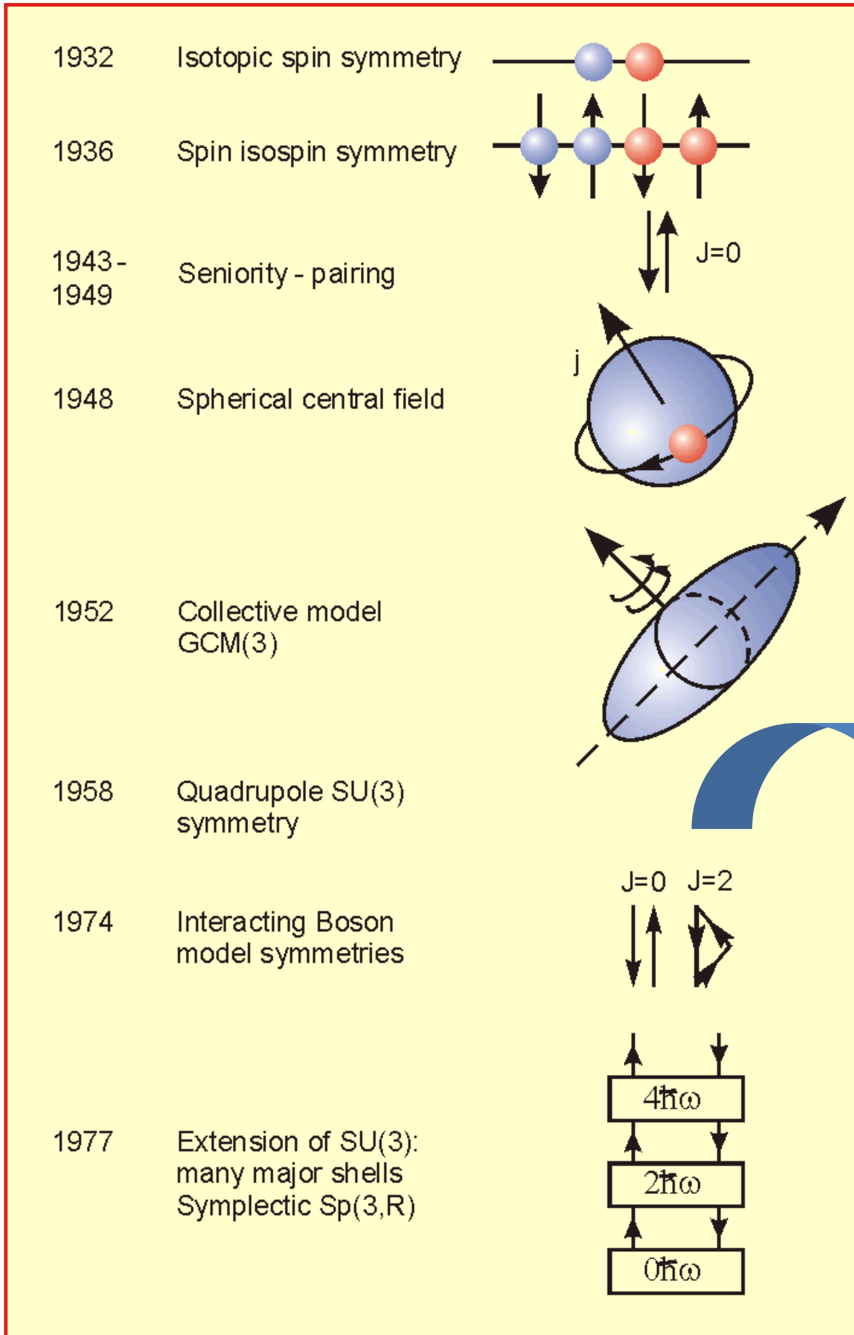
“Symmetry has been used as a guiding principle to create beauty and order in modeling the nuclear many-body system”

- Isotopic spin symmetry -SU(2)
  methods - SU(2) . Classification of many-nucleon configurations.
- Spin-isospin- SU(4) supermultiplet structure of nuclei
- The recognition of nucleon J=0 pair coupling scheme using group theoretical methods



J.P .Elliott
Proc.R.Soc.A245(1958)

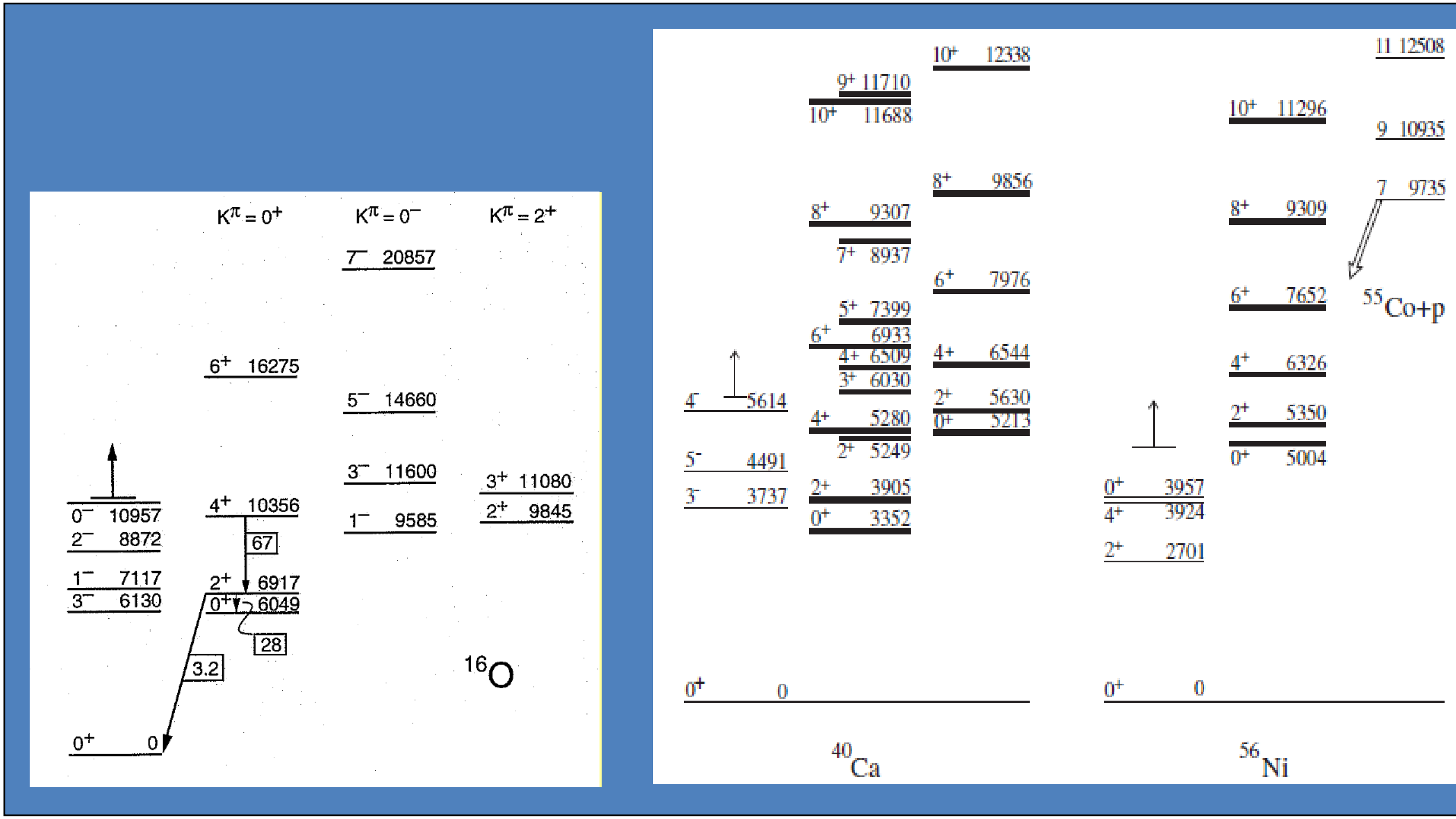
How do collective effects arise from individual particle behavior



A. Arima and F. Iachello, Ann.Phys. 1976,1978,1979

How do collective effects arise from individual particle behavior

Presence of deformed and superdeformed excitations in N=Z doubly-closed shell nuclei.



Need to extend the Elliott model to include mp-nh excitations

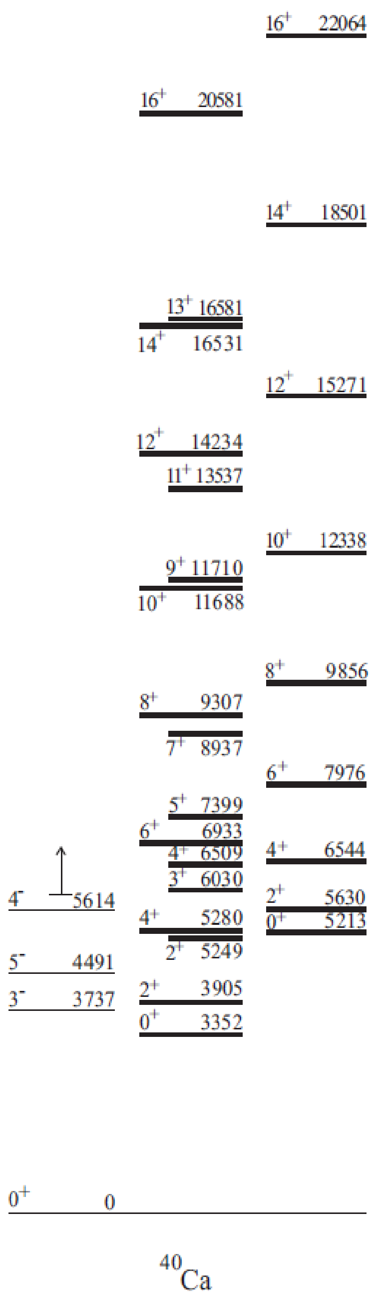
Collective states in “doubly-closed” shell nuclei: the example of ^{40}Ca

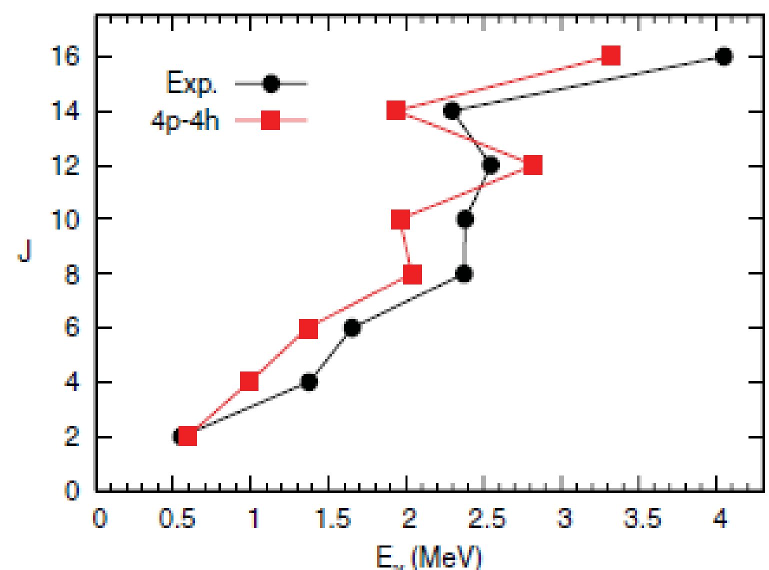
Multi-particle multi-hole excitations across the N=20, Z=20 ‘core’:

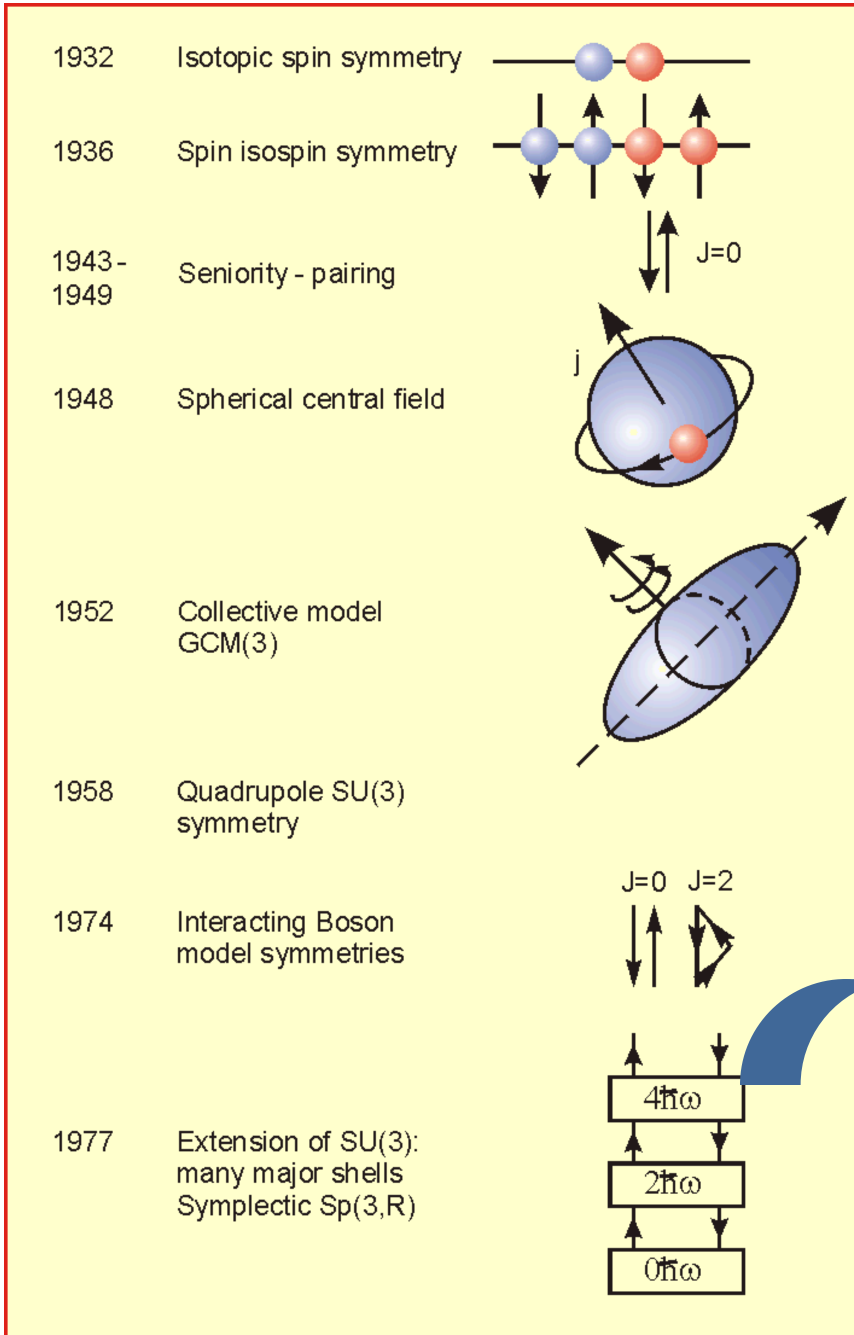
$2s_{1/2}$ $1d_{3/2}$ – full fp model space

Strongly correlated 4p-4h and 8p-8h structures: deformation -superdeformation

Caurier et al., PRC75(2007)

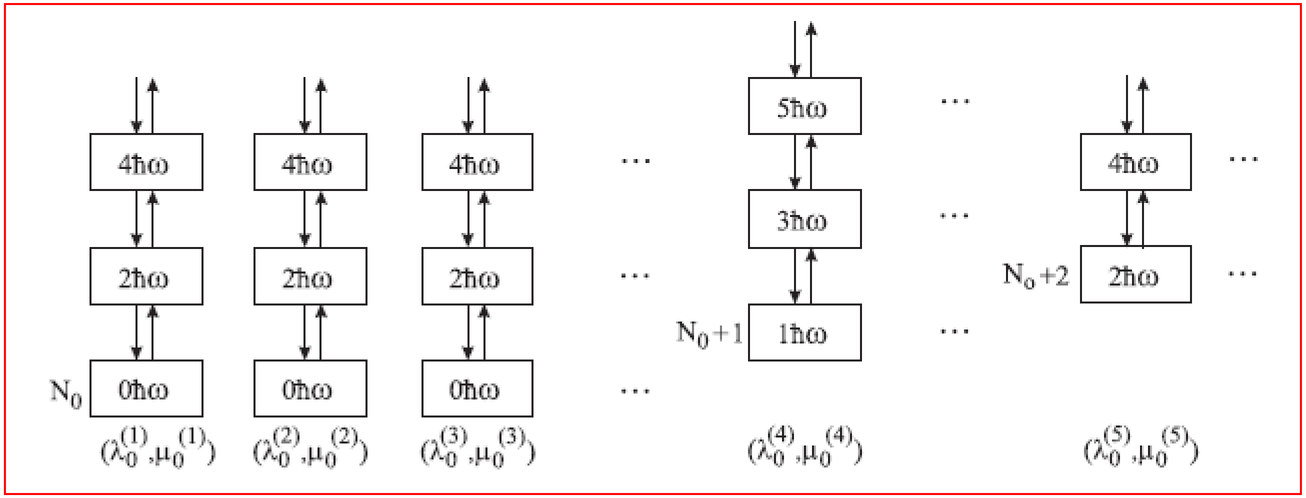






Group theoretical extension of SU(3) model: non-compact group Sp(3,R)
Also contains GCM(3) as subgroup

(Rosensteel and Rowe 1977),
Rowe et al., PRL(2006)



The vertical shells of the symplectic collective model, labeled by the number of oscillator quantum numbers of the SU(3) subgroup of the model [adopted from Rowe, Rept. Progr.Phys. 48, 1419(1985) and Carvallo et al., Nucl. Phys. A452,240(1986)]

Making use of the extension of the shell-model basis, to include many-particle many-hole excitations, leading to the Symplectic Group structure, the possibilities to describe collective degrees of freedom becomes possible.

Compared to the standard truncation methods handling a horizontal trunctions, considering in the early studies just a single major shell, and, with increasing computer power, a few of the adjacent shells, the Symplectic Shell Model approach considers a different truncation scheme by which the most important correlations are taken into account in a natural way.

(see talk of David Rowe)

A general way to extract intrinsic quadrupole deformation properties , independent of the theoretical model approach, starts from the construction of higher-order quadrupole invariant operators.

Kumar and Cline and Flaum, proposed the idea of making invariants out of products of the electric quadrupole operator E2 (quadratic, cubic, …) as early as 1972.

K.Kumar, PRL28,249(1972) D.Cline and C. Flaum, proc.of the Int.Conf. on Nuclear Structure using Electron Scattering, eds. K.Shoda ad H.Ui (Tohoku Univ. ,Sendai,1972),61

Construction of the higher-order moments of the quadrupole operator (E2) of second, cubic,… order.

$$\left\langle i \left| [E2 \otimes E2]_0^{(0)} \right| i \right\rangle$$

$$\left\langle i \left| \left[[E2 \otimes E2]^{(2)} \otimes E2 \right]_0^{(0)} \right| i \right\rangle$$

How can one determine these invariants for any given nuclear excited state.

The key points: 1

The E2 moments are “observables”.

If a sufficient number are experimentally determined, it is possible to determine the rotational invariants from the data.

$$\left\langle i \left| [E2 \otimes E2]_0^{(0)} \right| i \right\rangle = \frac{1}{\sqrt{5}} \frac{1}{2I_i + 1} \sum_t \left| \langle i \| E2 \| t \rangle \right|^2$$

$$\left\langle i \left| \left[[E2 \otimes E2]^{(2)} \otimes E2 \right]_0^{(0)} \right| i \right\rangle = \frac{(-1)^{2I_i}}{2I_i+1} \sum_{t,u} \langle i \| E2 \| u \rangle \langle u \| E2 \| t \rangle \langle t \| E2 \| i \rangle \times \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ I_i & I_u & I_t \end{array} \right\}.$$

Any theoretical model can evaluate those invariants.

The key points: (2)

These shape moments take a particular simple form in a body-fixed frame allowing to parameterize the nuclear deformation properties making use of two numbers only: the quadrupole moment and the deviation from axial symmetry in each eigenstate J,π

$$\langle E_{2,1}\rangle = \langle E_{2,1}\rangle = 0 \quad \langle E_{2,2}\rangle = \langle E_{2,-2}\rangle \equiv \frac{1}{\sqrt{2}}\langle Q.sin\delta\rangle$$

$$\langle E_{2,0}\rangle \equiv \langle Q.cos\delta\rangle$$

The quadrupole invariants reduce into a very simple form when making use of the the body-fixed principle axis system.

Data or nuclear model

$$\left\langle i \left| [E2 \otimes E2]_0^{(0)} \right| i \right\rangle = \frac{1}{\sqrt{5}} \frac{1}{2I_i + 1} \sum_t |\langle i \| E2 \| t \rangle|^2$$

$$\left\langle i \left| \left[[E2 \otimes E2]^{(2)} \otimes E2 \right]_0^{(0)} \right| i \right\rangle$$
$$= \frac{(-1)^{2I_i}}{2I_i+1} \sum_{t,u} \langle i \| E2 \| u \rangle \langle u \| E2 \| t \rangle \langle t \| E2 \| i \rangle$$
$$\times \left\{ \begin{array}{ccc} 2 & 2 & 2 \\ I_i & I_u & I_t \end{array} \right\}.$$

Principal axis form of invariants

$$= \frac{1}{\sqrt{5}} \langle Q^2 \rangle$$

$$= -\sqrt{\frac{2}{35}} \langle Q^3 \cos(3\delta) \rangle$$

Equivalent ellipsoid for the nucleus in state i = J,π

$$\mathrm{Q}^2 = (\tfrac{3}{4\pi} ZeR_0^2)^2 (\beta^2 + \mathcal{O}(\beta^3))$$

$$\mathrm{Q}^3 \cos(3\delta) = (\tfrac{3}{4\pi} ZeR_0^2)^3 (\beta^3 \cos(3\gamma) + \mathcal{O}(\beta^4))$$

Make use of any approach (spherical shell-model LSSM, MCSM approach, (Beyond) Mean-field approach, collective models,..
(recent papers H. Nadidja, F. Nowacki et al., PRC96,034312 (2017),
T. Schmidt, K.Heyde et al., PRC96,014302(2017) and refs. therein)

Use experimental results of the reduced E2 matrix elements: Coulomb-excitation , lifetime data, … to calculate the invariants and the extracted deformation results.

Very recent: studies within the finite-temperature auxiliary-field Quantum Monte-Carlo method (in short Shell-Model Monte-Carlo or SMMC method : Koonin, Dean and Langanke, Repts.Phys. 278,1 (1978): Alhassid, Bertsch, Gilbreth(PRL 113, 262503(2014), arXiv 10 October 2017, 1710.00072v2)

Shape coexistence has evolved from an exotic rarity (50's) to its current status throughout the nuclear mass region.

Unified way to capture low-lying intruder states and regions of "deformation

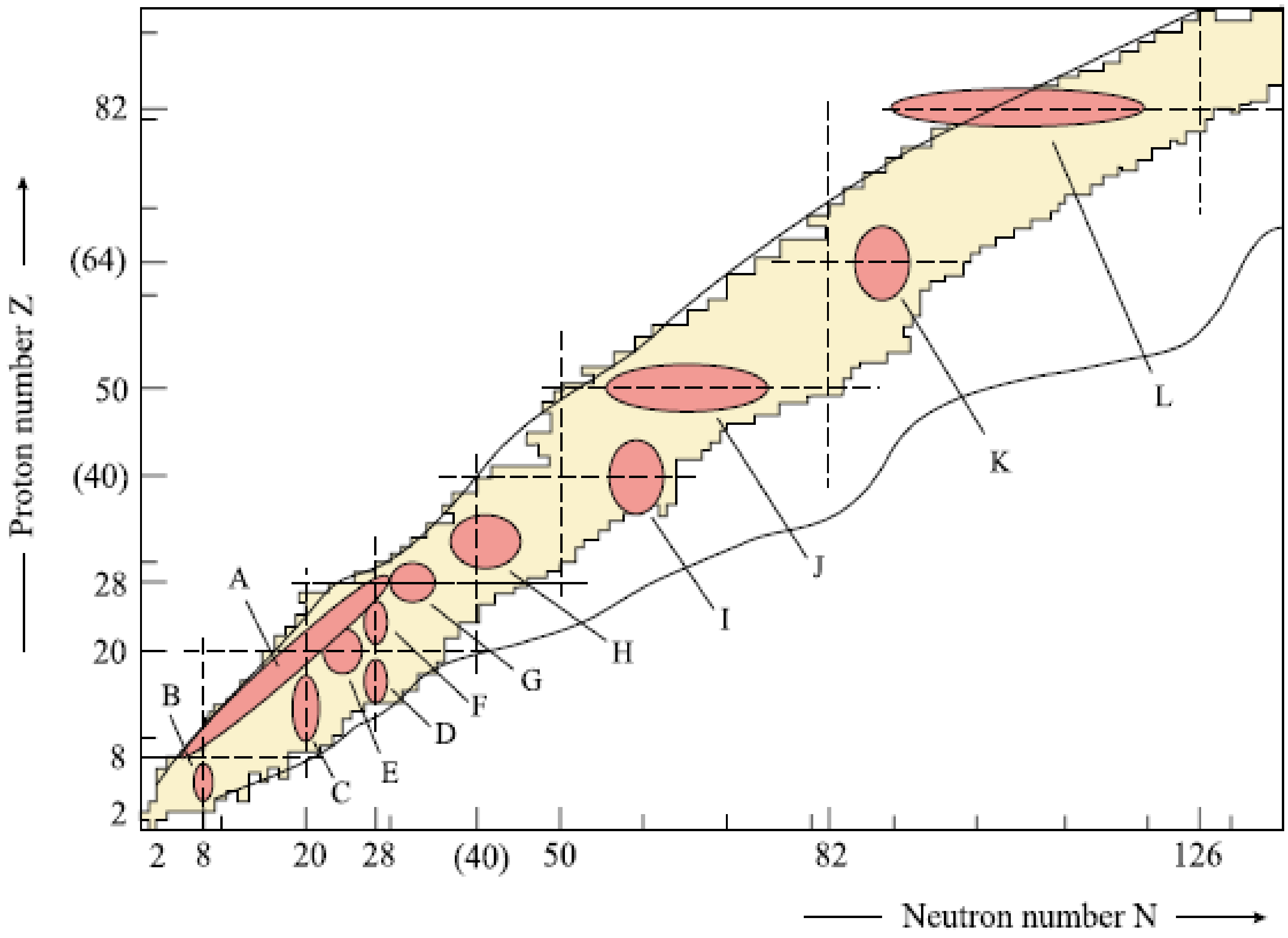
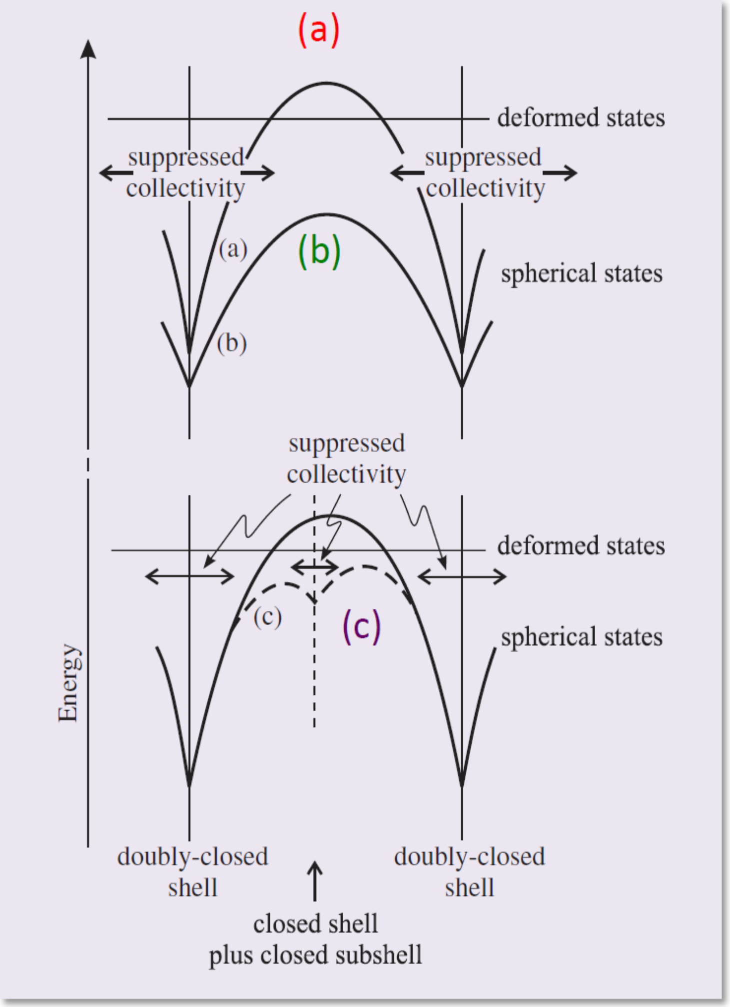


Figure from K. Heyde and J.L.Wood Rev.Mod.Phys. 83,1467 (2011)

Shape coexistence at shell and subshell gaps: the suppression of collectivity



Shape coexistence in regions such as:

(a) ^{32}Mg

(b) ^{116}Sn

(c) ^{90}Zr

Figure from K. Heyde and J.L.Wood, Rev. Mod. Phys. 83, 1467 (2011)

Thanks a lot to my long-term collaborator J.L.Wood spanning more than 35 years

The theory groups at the University of Ghent, Leuven, Köln, GANIL, Sevilla, and many more.

The inventive and hard work by many groups doing the experiments that allowed to obtain the keys to explore yet new regions in the nuclear landscape and with data that have been showing the early roads, and where to take exits leading to better views of the landscape.