Shape Coexistence; A Shell Model View

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ESNT Workshop

Saclay, November 16-19, 2015

Outline

- Introduction
- Collectivity in the Laboratory Frame. Elliott's SU(3) and its variants
- ^{40}Ca; Shape Coexistence
- ^{72}Kr; Shape Entanglement?
- Conclusions

Why Shell Model?

- Because to connect rigorously the free space nucleon nucleon interaction with the experimental spectroscopic data has been the Holy Grail of Nuclear Physics since its inceptions.
- And, indeed, the SM results relate directly to observables, without breaking symmetries beyond translational invariance

Why Shell Model?

- The SM is an approximate solution to the full many body problem using effective interactions in a restricted set of orbits of an underlying spherical mean field (the valence space).
- The two intertwined ingredients of a SM calculation are therefore the valence space and the effective interaction (which may naturally be of more than two-body rank. Indeed performant algorithms and codes are necessary to cope with the huge dimensions of the problem.

Why Nuclear Shape?

- Because we are still heirs of the semiclassical liquid-drop like models
- The very concept of shape requires to break the rotational (and reflection) invariance, or, equivalently to define an intrinsic reference frame. But even if the symmetry is broken, we need to rely on semiclassical models, liquid-drop like, to define a vocabulary which describes properties akin to the concept of shape.
- The surface of a drop can be expressed in the basis of the spherical harmonics $Y_{\lambda,\mu}(\theta,\phi)$. The coefficients of the development, $\alpha_{\lambda,\mu}$, are the shape parameters. To speak about nuclear shape, we need a protocol to extract the best information about these intrinsic shape parameters from the nuclear wave functions in the laboratory frame.

Elliott's SU3

- **The description of the nuclear deformation and hence the nuclear shape in the laboratory frame was found by Elliott. Using the fact that SU3 is a symmetry of the spherical harmonic oscillator (HO), and restricting the two body interaction to a quadrupole-quadrupole force, he was able to solve analytically the nuclear many body problem using the elegant and powerful mathematical techniques of group theory.**

Elliott's SU3

- **Not only $J(J+1)$ spectra were obtained without breaking the rotational invariance, furthermore the notion of an intrinsic state appeared associated to the choice of the chain of subgroups of SU(3) used to label the eigenfunctions of the problem: O(3)-U(1) for the physical states and SU(2)-U(1) for the intrinsic ones. In the latter case, a new quantum number emerge, the intrinsic quadrupole moment, Q_0, the sought shape parameter.**

Shape Parameters; The Case of Quadrupole Deformation

- **From the value of Q_0 one can get the deformation parameter β using different recipes, for instance:**

$$Q_0 = \frac{3}{\sqrt{5\pi}} R^2 Z \,(1 + 0.16\, \beta)\, \beta \tag{1}$$

- **If the nucleus is not axially symmetric, the situation becomes more convoluted, because now we need to recover two shape parameters, β and γ. The former can in most cases be extracted from the B(E2)'s as in the axial case, but for γ we have to resort to other expediencies. Davidov and Filipov use the collective model to extract the values of γ from the B(E2)values of the transitions between the yrast and the γ bands.**

Shape Parameters; The Case of Quadrupole Deformation

- **Another possibility is to rely on the use of the expectation values of scalars constructed with the quadrupole operator like $(Q_2 \times Q_2)^0$ or $(Q_2 \times Q_2 \times Q_2)^0$ as proposed by Kumar. These expectation values can be written in terms of the shape parameters. Finally, one could use a basis in the intrinsic frame to perform laboratory frame calculations as in the MCSM (Monte Carlo Shell Model), and keep track of the shape parameter content of the physical solutions.**

Many Particles and Orbits around the Fermi Level

- To solve the many body problem to spectroscopic accuracy, Large Scale Shell Model calculations have proven very successful when affordable.
- In other cases, approximations have to be made, either of physical (IBM) or mathematical (MCSM) nature
- Only recently, Beyond Mean Field calculations using Energy Density Functionals have been pushed to quantitative spectroscopy. However, many things that are trivial in LSSM, like the correct treatment of all the pairing channels or the inclusion of triaxial and higher multipolarity degrees of freedom, become extremely painful for BFM.

Where?

Physically sound and tractable SM valence spaces:

- **The classical 0$\hbar\omega$ spaces *p*, *sd*, and *pf* shells can be treated exactly.**
- **Nuclei (or states) at the *p*-*sd* and *sd*-*pf* borders, can be described to a very good approximation *e. g.* Low lying deformed and super deformed banda in ^{40}Ca.**
- **Neutron rich nuclei with protons in the *sd*-shell and neutrons in the *pf*-shell can be treated exactly as well *e. g.* ^{32}Mg, ^{34}Si, ^{42}Si, ^{44}S.**
- **The space r3g (1p$_{3/2}$, 1p$_{1/2}$, 0f$_{5/2}$, 0g$_{9/2}$), is also solved exactly. But its physical relevance is limited to a rather small part of its natural span, *e. g.* ^{76}Ge, ^{82}Se.**

Where?

Physically sound and tractable SM valence spaces

- **The space r3gd ($1p_{3/2}$, $1p_{1/2}$, $0f_{5/2}$, $0g_{9/2}$ $1d_{5/2}$) for the neutrons and *pf* for the neutrons, for the very neutron rich isotopes from Calcium to Germanium.** *e. g.* ^{68}**Ni,** ^{64}**Cr,** ^{78}**Ni,** ^{80}**Zn.**
- **The space** *sdg* **around** ^{100}**Sn**
- **The space r4h comprised between N=Z=50 and N=Z=82 for a small subset of the nuclei it encompasses; the Sn, Te , Xe and Ba isotopes up to N=82.**
- **Protons in r4h and neutrons in r5i; the very neutron rich Sn, Te , Xe and Ba isotopes, beyond N=82.**
- **Around** ^{208}**Pb**

Many Particles and Orbits around the Fermi Level

More is different:

- **Indeed, since you can treat more and heavier nuclei, but in addition, because some of these nuclei exhibit collective features which are better developed than in their *sd* shell Elliott's like precursors**
- **And because their description was until now restricted to the mean field approaches**
- **Our approach to the SM relies on the Monopole-Multipole decomposition of the effective Hamiltonian**

The Spherical Mean Field (Monopole Hamiltonian)

$$\mathcal{H}_m = \sum n_i \epsilon_i + \sum \frac{1}{(1+\delta_{ij})} \overline{V}_{ij}\, n_i (n_j - \delta_{ij})$$

the coefficients $\overline{V}$ are angular averages of the two body matrix elements, or centroïds of the two body interaction:

$$\overline{V}_{ij} = \frac{\sum_J V_{ijij}^J [J]}{\sum_J [J]}$$

the sums running over Pauli allowed values.

The Spherical Mean Field (Monopole Hamiltonian)

This can be written as well as:

$$\mathcal{H}_m = \sum_i n_i \left[\epsilon_i + \sum_j \frac{1}{(1+\delta_{ij})} \overline{V}_{ij} \left(n_j - \delta_{ij}\right) \right]$$

Thus

$$\mathcal{H}_m = \sum_i n_i \;\; \hat{\epsilon}_i(\left[n_j\right])$$

We call these $\hat{\epsilon}_i(\left[n_j\right])$ effective single particle energies (ESPE)

Effective Single Particle Energies

They give the evolution of the underlying (non observable) spherical mean field (aka, shell evolution) as we add particles in the valence space, as well as the variations of the spherical mean field in a single nucleus for states which have different configurations.

They are the control parameter for the nuclear dynamics, given the universality of the nuclear multipole hamiltonian.

Monopole anomalies of the realistic NN interactions

They are the more blatant in the neutron-neutron interaction; for instance not producing a magic ^{48}Ca, or the location of the drip line in the Oxygen isotopes

Notably, their monopole neutron proton tensor part is correct, and the spin orbit splittings well accounted for.

The blame probably rest in missing residual three body effects

The Nuclear Correlators (Multipole Hamiltonian)

- **The multipole hamiltonian is responsible for the collective nuclear behavior. It is universal and well given by the realistic NN interactions. Its main components are:**
- **BCS-like isovector and isoscalar pairing. When pairing dominates, as in the case of nuclei with only neutrons (or only protons) on top of a doubly magic nucleus, it produces nuclear superfluids.**
- **Quadrupole-Quadrupole and Octupole-Octupole terms of very simple nature ($r^\lambda Y_\lambda \cdot r^\lambda Y_\lambda$) which tend to make the nucleus deformed. In this limit, the pairing correlations mainly show up as responsible for the moment of inertia of the nuclear rotors.**

Why do the quadrupole correlations thrive in the nucleus?

- The fact that the spherical nuclear mean field is close to the HO has profound consequences, because the dynamical symmetry of the HO, responsible for the accidental degeneracies of its spectrum, is SU(3), among whose generators it is the quadrupole operator.
- When valence protons an neutrons occupy the degenerate orbits a major oscillator shell, and for an attractive Q·Q interaction, the many body problem has an analytical solution in which the ground state of the nucleus is maximally deformed (Elliott's model)

Why do the quadrupole correlations thrive in the nucleus?

- **In cases when both valence neutrons and protons occupy quasi-degenerate orbits with Δj= 2 and Δj=2, including j=p+1/2 (Quasi-SU3), or quasi-spin multiplets (Pseudo-SU3)**
- **For example, $0f_{7/2}$ and $1p_{3/2}$, or $0g_{9/2}$ $1d_{5/2}$ and $2s_{1/2}$ form Quasi-SU3 multiplets and $0f_{5/2}$, $1p_{3/2}$ and $1p_{1/2}$ a Pseudo-SU3 triplet**

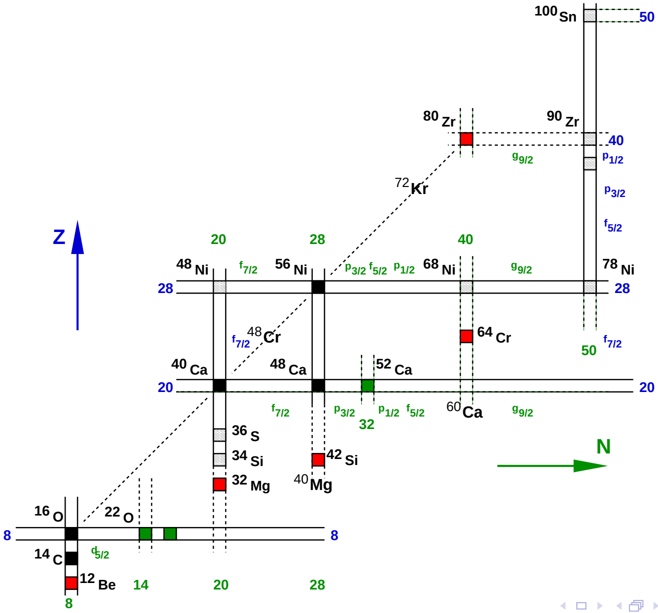
Quadrupole dominance in the Quasi + Pseudo SU3 frame

- The Quasi + Pseudo SU3 or Quasi + Quasi SU3 scheme plus the monopole field provide a SM toolkit to locate deformed structures in the (N, Z, E^*) landscape.
- We shall examine two model spaces; sd-pf and pf-sdg and study the behavior of np-nh configurations across N,Z=20 or N,Z=40
- In both cases the n particles sit in Quasi-SU3 orbits and the n holes in Pseudo-SU3, or in Quasi-SU3 as well, thus maximizing their quadrupole moments and, a fortiori, their quadrupole correlation energy.
- Depending on the doings of the monopole field, this can produce shape coexistence, shape transitions, shape mixing, islands of inversion etc.

Typical Values

- The maximum single particle q_0's are 2p$\times$b^2 for SU(3) and (2p-1/2)$\times$b^2 for Quasi-SU(3); p being the principal HO quantum number $E = \hbar\omega(p + 3/2)$.
- The intrinsic quadrupole moment of a normal deformed (ND) nucleus in the *pf*-shell (^{48}Cr) is about 120 fm^2. The deformation β should be 0.3 in this case
- For a K=0 band, in the rotational limit,
  Q_0= –3.5 $Q_{spec}(2^+)$ and
  Q_0^2= 50.2 $\times$ B(E2)($2^+ \rightarrow 0^+$)
- b^2 values range from 3.5 fm^2 in ^{40}Ca to 4.5 fm^2 in ^{72}Kr

Landscape of medium mass exotica

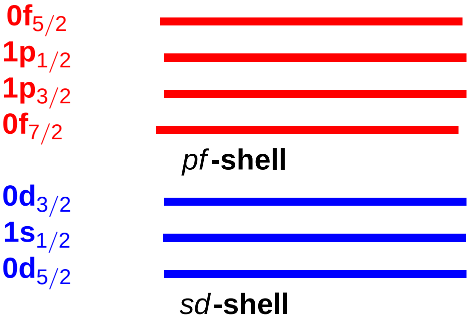


^{48}Cr a Quasi-SU3 paradigm

- **Four protons and four neutrons in Quasi-SU3 amount to Q_0= (4$\times$5.5 + 4$\times$2.5 +3)$\times$b^2**
- **Which gives about 120 fm^2, with effective charges 1.5 and 0.5**
- **In quite good agreement with experiment and with a full *pf*-shell calculation using the KB3G interaction, even if overshooting the quadrupole moment by 10%**
- **This gives us a first hint of the resilience of the quadrupole properties to deviations of the spherical mean field from the "ideal" SU3 one**

Extreme Shape Coexistence in ^{40}Ca

In the valence space of two major shells

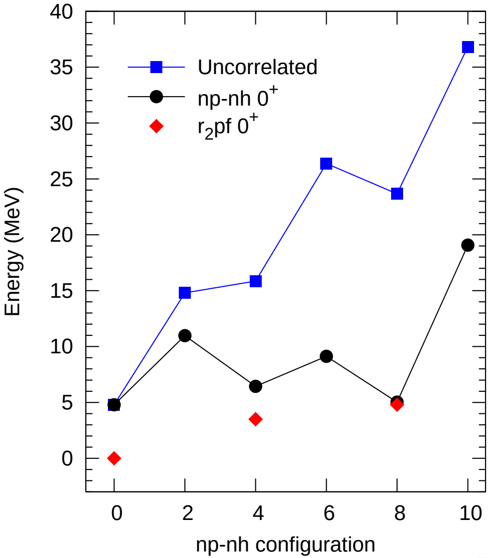


Spherical, Deformed and Superdeformed states

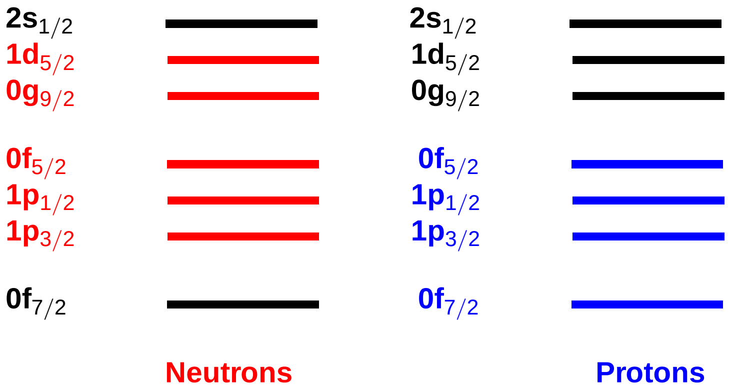
The relevant configurations in ^{40}Ca are:

- **[sd]^{24} 0p-0h, SPHERICAL**
- **[sd]^{20} [pf]^{4} 4p-4h, DEFORMED; Q_0=29 b^2**
- **[sd]^{16} [pf]^{8} 8p-8h, SUPERDEFORMED: Q_0=48 b^2**
- **The correlation energies go roughly as Q_0^2**

The correlation energies, or why Shapes Coexist



The valence space adequate for the N=40 isotones contains all these ingredients as well



For N=Z, ^{56}Ni provides a good core. Approaching N=2Z, one should rather switch to ^{48}Ca

Quadrupole dominance in the Quasi + Pseudo SU3 frame

- **The Quasi + Pseudo SU3 or Quasi + Quasi SU3 scheme plus the monopole field provide a SM toolkit to locate deformed structures in the (N, Z, E^*) landscape as well.**
- **The ground states of the N=Z nuclei between ^{68}Se and ^{92}Pd, (and their neighbors) are dominated by configurations with np-nh jumps across N=Z=40, which may produce oblate and prolate shapes, and hence, sometimes shape related phenomena.**
- **Why? Because the n particles sit in Quasi-SU3 orbits and the n holes in Pseudo-SU3, thus maximizing their quadrupole moments and, a fortiori, their quadrupole correlation energy, which suffices to beat by large the monopole energy cost of crossing the N=Z=40 gap.**

Intrinsic Quadrupole moments for Pseudo (r3g) and Quasi-SU3 (gds): prolate states

The most favorable configurations from the quadrupole point of view are:

^{72}Kr

4p-4h; Q_0= $\pm$60 b^2 8p-8h; Q_0= 73 b^2 12p-12h; Q_0= 74 b^2

^{76}Sr

4p-4h; Q_0= 51 b^2 8p-8h; Q_0= 77 b^2 12p-12h; Q_0= 79 b^2

^{80}Zr

8p-8h; Q_0= 72 b^2 12p-12h; Q_0= 83 b^2 16p-16h; Q_0= 85 b^2

Monopole *vs* Quadrupole

- **We have recently shown that these quadrupole moments are resilient to departures of the SPE from their degenerated limit (Zuker *et al.* PRC 92, 2015)**
- **The key point here is that the quadrupole energy gains grow with the square of the quadrupole moment whereas the monopole losses are at most proportional to the number of particle-hole jumps**
- **In ^{76}Sr and ^{80}Zr the deformed configurations, 8p-8h and 12p-12h win comfortably. In ^{72}Kr the 4p-4h prolate and the oblate solutions (oblate meaning $(0g_{9/2})^4$ instead of $(gds)^4$) are degenerated as we shall discuss next.**
- **From Q_0 one can deduce the B(E2)'s. The $2^+ \to 0^+$ are equal to $Q_0{}^2/50.3$ and the $4^+ \to 2^+$ a factor 1.43 larger.**

Comparing with experiment

Using b^2=4.5 fm^2 we obtain the following B(E2) values:

- **^{72}Kr; $2^+ \rightarrow 0^+$; 1470 e^2fm^4; $4^+ \rightarrow 2^+$; 2100 e^2fm^4**
- **^{76}Sr; $2^+ \rightarrow 0^+$; 2380 e^2fm^4; $4^+ \rightarrow 2^+$; 3410 e^2fm^4**
- **^{80}Zr; $2^+ \rightarrow 0^+$; 2800 e^2fm^4; $4^+ \rightarrow 2^+$; 4000 e^2fm^4**

To compare with the available experimental results:

- **^{72}Kr; $2^+ \rightarrow 0^+$; 810(150) e^2fm^4; $4^+ \rightarrow 2^+$; 2720(550) e^2fm^4**
- **^{76}Sr; $2^+ \rightarrow 0^+$; 2200(270) e^2fm^4**
- **^{80}Zr; no data yet**

Excellent agreement except for the $2^+ \rightarrow 0^+$ of ^{72}Kr. But this is a blessing in disguise because it led us to understand better the prolate oblate coexistence in this nucleus.

^{72}Kr, a case of full prolate oblate mixing

- It is common lore to speak of prolate-oblate or prolate-spherical coexistence when an excited 0^+ state appears at very low energy. This is the case in ^{72}Kr, whose first excited state is a 0^+ at 671 keV followed by a 2^+ at 710 keV. The very large B(E2) of the transition $4^+ \rightarrow 2^+$ strongly suggest that the 2^+ belongs to a prolate band which extends up to J=16^+. But, if so, where is the band head?
- If we follow down the J(J+1) sequence from the upper part of the band we should expect it 250 keV below the 2^+, which is very close to the experimental excitation energies of the 2^+ in ^{76}Sr and ^{80}Kr. Obviously the distortion must be due to the mixing of the prolate band-head with a near lying oblate state.

^{72}Kr, prolate oblate mixing, a (very) simple model

- **The first element to take into account is that the oblate and prolate 4p-4h states do not mix directly;** *i.e.* $\langle p|H|o\rangle$ **= 0**
- **The mixing should then proceed through 2p-2h or 6p-6h states. Lets take these to be represented by an auxiliary state $|I\rangle$, and further assume that it lies at about ΔE=4 MeV (as our calculations show) and that its coupling to both prolate and oblate states is equal to δ. Taking them degenerated for simplicity, the mixing matrix reads:**
- $$\begin{pmatrix} 0 & 0 & \delta \\ 0 & 0 & \delta \\ \delta & \delta & \Delta E \end{pmatrix}$$

^{72}Kr, prolate oblate mixing, a (very) simple model

- **The mixing can proceed through a cloud of N states, then the matrix is**
- $$\begin{pmatrix} 0 & 0 & \beta & \beta & \beta & \dots \\ 0 & 0 & \beta & \beta & \beta & \dots \\ \beta & \beta & \Delta E & 0 & 0 & \dots \\ \beta & \beta & 0 & \Delta E & 0 & \dots \\ \beta & \beta & 0 & 0 & \Delta E & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}$$
- **Which has the same two lowest eigenvalues and eigenvectors if** $\delta = \sqrt{N}\ \beta$

^{72}Kr, prolate oblate mixing, a (very) simple model

- For $\delta \sim$ 1 MeV, which is a sensible choice, the eigenvalues are: –0.5 MeV, 0.0 MeV and +4.5 MeV. They fit nicely the experimental energies.
  The eigenstates corresponding to the two lower eigenvalues are:
  $|0^+_1\rangle$ = 43% $|p\rangle$ + 43% $|o\rangle$ + 16% $|I\rangle$ and
  $|0^+_2\rangle$ = 50% $|p\rangle$ + 50% $|o\rangle$
- Therefore, the B(E2)($2^+ \rightarrow 0^+_1$) will be approximately one half of the expected value for the prolate band in full accord with the experimental data
- What is the shape of an object which is an even mixture of prolate and oblate? What is the nature of this mixing of shapes? Or should we speak of a shape entangled state?

Conclusions

- Shape coexistence is a consequence of the interplay between the spherical mean field and the multipole correlators
- In valence spaces comprising two major oscillator shell LSSM calculations explain shape related phenomena like coexistence, mixing and entanglement.