

The Shell Model: An Unified Description of the Structure of the Nucleus

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- **Quadrupole Collectivity; SU3 and its variants**
- **Applications: ^{40}Ca and ^{48}Cr**

The SU3 symmetry of the harmonic oscillator

The mechanism that produces permanent deformation and rotational spectra in nuclei is much better understood in the framework of the SU(3) symmetry of the isotropic harmonic oscillator and its implementation in Elliott's model. The basic simplification of the model is threefold; i) the valence space is limited to one major HO shell; ii) the monopole hamiltonian makes the orbits of this shell degenerated and iii) the multipole hamiltonian only contains the quadrupole-quadrupole interaction. This implies (mainly) that the spin orbit splitting and the pairing interaction are put to zero. Let's then start with the spherical HO which in units $m=1$ $\omega=1$ can be written as:

$$H_0 = \frac{1}{2}(p^2 + r^2) = \frac{1}{2}(\vec{p} + i\vec{r})(\vec{p} - i\vec{r}) + \frac{3}{2}\hbar = \hbar(\vec{A}^\dagger \vec{A} + \frac{3}{2})$$

The SU3 symmetry of the harmonic oscillator

$$\vec{A}^\dagger = \frac{1}{\sqrt{2\hbar}}(\vec{p} + i\vec{r}) \quad \vec{A} = \frac{1}{\sqrt{2\hbar}}(\vec{p} - i\vec{r})$$

which have bosonic commutation relations. H_0 is invariant under all the transformations which leave invariant the scalar product $\vec{A}^\dagger \vec{A}$. As the vectors are three dimensional and complex, the symmetry group is U(3). We can build the generators of U(3) as bi-linear operators in the A's. The anti-symmetric combinations produce the three components of the orbital angular momentum L_x , L_y and L_z , which are on turn the generators of the rotation group O(3). From the six symmetric bi-linears we can retire the trace that is a constant; the mean field energy. Taking it out we move into the group SU(3). The five remaining generators are the five components of the quadrupole operator:

The SU3 symmetry of the harmonic oscillator

$$q_{\mu}^{(2)} = \frac{\sqrt{6}}{2\hbar} (\vec{r} \wedge \vec{r})_{\mu}^{(2)} + \frac{\sqrt{6}}{2\hbar} (\vec{p} \wedge \vec{p})_{\mu}^{(2)}$$

The generators of SU(3) transform single nucleon wavefunctions of a given p (principal quantum number) into themselves. In a single nucleon state there are p oscillator quanta which behave as $l=1$ bosons. When we have several particles we need to construct the *irreps* of SU(3) which are characterized by the Young's tableaux (n_1, n_2, n_3) with $n_1 \geq n_2 \geq n_3$ and $n_1 + n_2 + n_3 = Np$ (N being the number of particles in the open shell). The states of one particle in the p shell correspond to the representation $(p, 0, 0)$. Given the constancy of Np the *irreps* can be labeled with only two numbers. Elliott's choice was $\lambda = n_1 - n_3$ and $\mu = n_2 - n_3$. In the cartesian basis we have; $n_x = a + \mu$, $n_y = a$, and $n_z = a + \lambda + \mu$, with $3a + \lambda + 2\mu = Np$.

The SU3 symmetry of the harmonic oscillator

The quadratic Casimir operator of SU(3) is built from the generators

$$\vec{L} = \sum_{i=1}^N \vec{l}(i) \quad Q_{\alpha}^{(2)} = \sum_{i=1}^N q_{\alpha}^{(2)}(i)$$

as:

$$C_{SU(3)} = \frac{3}{4}(\vec{L} \cdot \vec{L}) + \frac{1}{4}(Q^{(2)} \cdot Q^{(2)})$$

and commutes with them. With the usual group theoretical techniques, it can be shown that the eigenvalues of the Casimir operator in a given representation (λ, μ) are:

$$C(\lambda, \mu) = \lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)$$

Elliott's Model

Once these tools ready we come back to the physics problem as posed by Elliott's hamiltonian

$$H = H_0 + \chi(Q^{(2)} \cdot Q^{(2)})$$

which can be rewritten as:

$$H = H_0 + 4\chi C_{SU(3)} - 3\chi(\vec{L} \cdot \vec{L})$$

The eigenvectors of this problem are thus characterized by the quantum numbers λ , μ , and L. We can choose to label our states with these quantum numbers because O(3) is a subgroup of SU(3) and therefore the problem has an analytical solution:

Elliott's Model

$$E(\lambda, \mu, L) = \hbar\omega\left(p + \frac{3}{2}\right) + 4\chi(\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)) - 3\chi L(L + 1)$$

This final result can be interpreted as follows: For an attractive quadrupole quadrupole interaction ($\chi < 0$) the ground state of the problem pertains to the representation which maximizes the value of the Casimir operator, and this corresponds to maximizing λ or μ (the choice is arbitrary). If we look at that in the cartesian basis, this state is the one which has the maximum number of oscillator quanta in the Z-direction, thus breaking the symmetry at the intrinsic level. We can then speak of a deformed solution even if its wave function conserves the good quantum numbers of the rotation group, i.e. L and L_z .

Elliott's Model

$$E(\lambda, \mu, L) = \hbar\omega\left(p + \frac{3}{2}\right) + 4\chi(\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)) - 3\chi L(L + 1)$$

For this one (and for every) (λ, μ) representation, there are different values of L which are permitted, for instance for the representation $(\lambda, 0)$ $L=0,2,4 \dots \lambda$. And their energies satisfy the $L(L+1)$ law, thus giving the spectrum of a rigid rotor. The problem of the description of deformed nuclear rotors is thus formally solved.

$E_{\text{level}}^{\#}$	J^{π}	$T_{1/2}$	XREF	Comments
0.0	0+	stable	ABCDEFGHIJ KLMNOPQR	
1368.672 5	2+	1.33 ps 6	A CDE GHIJ KLMNO Q	$\mu=+1.02 4$; $Q=-0.166 6$ J^{π} : E2 to 0+.
4122.889 12	4+	22 fs 2	A C E HIJ KLM P R	$\mu=+1.6 12$ J^{π} : E2 to 2+, L=4 in (p,p')
4238.24 3	2+	41 fs 4	A CDE HIJ KLM OP R	$\mu=+1.2 4$ J^{π} : E2 to 0+.
5235.12 4	3+	61 fs 7	A C HIJ KLM R	J^{π} : M1+E2 to 2+, L=3 in
6010.84 4	4+	49 fs 5	C HIJ KLM OP R	$\mu=+2.0 16$ J^{π} : γ 's to 0+ and 4+.
6432.30 11	0+	53 fs 8	HIJ K O R	J^{π} : L=0 in (p,p').
7349.00 3	2+	6 fs 2	C HIJ KLM O	J^{π} : E2 to 0+.
7555.04 15	1-	270 fs 55	HIJ KLM	J^{π} : E1 to 0+.
7616.47 4	3-	890 fs 140	C HIJ KL O	J^{π} : L=3 in (p,p'), (α,γ).
7747.51 9	1+	10 fs 3	HIJ L	J^{π} : M1 to 0+.
7812.35 11	5+	20 fs 4	C HIJ M R	J^{π} : From (α,γ).
8114.2 20	6+	3.6 fs 10	HI M R	J^{π} : L=6 in (p,p').
8357.98 13	3-	56 fs 8	HIJ LM O R	J^{π} : L=0 in (p,p').
8437.31 15	1-	10 fs 2	HIJ	J^{π} : E1 to 0+.
8439.36 4	4+	3.8 fs 11	C HIJ LM	J^{π} : log ft=3.93 from 4+, (α,γ)
8654.53 15	2+	8.2 fs 21	HIJ LM R	J^{π} : L=2 in (p,p'), γ to 0+.
8864.29 9	2-	4.4 fs 15	HIJ LM	J^{π} : L=1 in ($^3\text{He,d}$) and (^3He)
9003.34 9	2+	7.6 fs 14	HIJ M O	J^{π} : γ 's to 0+ and 4+, L=2
9145.99 15	1-		HI	J^{π} : L=1 in (p,p').

Intrinsic States

We can describe the intrinsic states and its relationship with the physical ones using another chain of subgroups of $SU(3)$. The one we have used until now is; $SU(3) \supset O(3) \supset U(1)$ which corresponds to labeling the states as $\Psi([\tilde{f}] (\lambda\mu) LM)$. $[\tilde{f}]$ is the representation of $U(\Omega)$ conjugate of the $U(4)$ spin-isospin representation which guarantees the antisymmetry of the total wave function. For instance, in the case of ^{20}Ne , the fundamental representation $(8,0)$ (four particles in $p=2$) is fully symmetric, $[\tilde{f}]=[4]$, and its conjugate representation in the $U(4)$ of Wigner $[1, 1, 1, 1]$, fully antisymmetric.

Intrinsic States

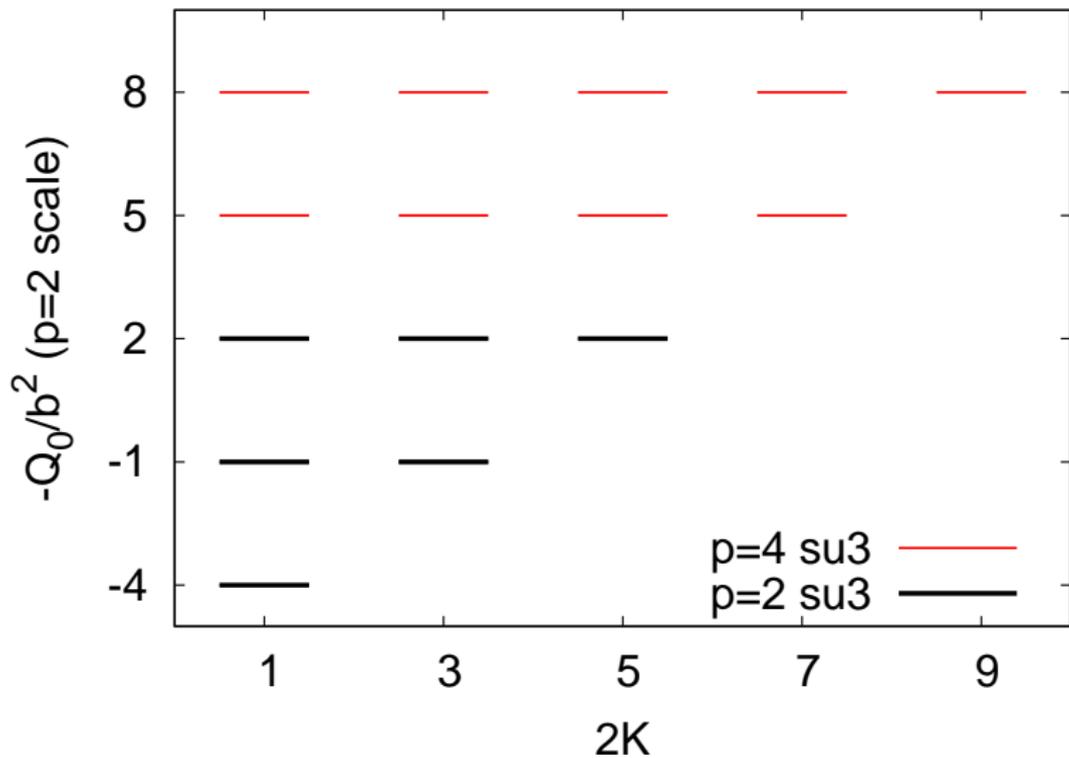
The other chain of subgroups, $SU(3) \supset SU(2) \supset U(1)$, does not contain $O(3)$ and therefore the total orbital angular momentum is not a good quantum number anymore. Instead we label the wave functions as; $\Phi([\tilde{f}](\lambda\mu)q_0\Lambda K)$, where q_0 is a quadrupole moment whose maximum value is $q_0 = 2\lambda + \mu$ related to the intrinsic quadrupole moment, $Q_0 = q_0 + 3$. K is the projection of the angular momentum on the Z-axis and Λ is an angular momentum without physical meaning. Both representations provide a complete basis, therefore it is possible to write the physical states in the basis of the intrinsic ones.

Actually, the physical states can be projected out of the intrinsic states with maximum quadrupole moment as:

$$\Psi([\tilde{f}](\lambda\mu)LM) = \frac{2L+1}{a(\lambda\mu KL)} \int D_{MK}^L(\omega) \Phi_{\omega}([\tilde{f}](\lambda\mu)(q_0)_{max} \Lambda K) d\omega$$

Remarkably, this is the same kind of expression used in the unified model; the Wigner functions D being the eigenfunctions of the rigid rotor and the intrinsic functions the solutions of the Nilsson model.

SU3 intrinsic states



Elliott's Model

Elliott's model was initially applied to nuclei belonging to the *sd*-shell that show rotational features like ^{20}Ne and ^{24}Mg . The fundamental representation for ^{20}Ne is (8,0) and its intrinsic quadrupole moment $19 \text{ b}^2 \approx 60 \text{ efm}^2$. For ^{24}Mg we have (8,4) and $23 \text{ b}^2 \approx 70 \text{ efm}^2$. To compare these figures with the experimental values we need to know the transformation rules from intrinsic to laboratory frame quantities and vice versa. In the Bohr Mottelson model these are:

$$Q_0(s) = \frac{(J+1)(2J+3)}{3K^2 - J(J+1)} Q_{\text{spec}}(J), \quad K \neq 1$$

$$B(E2, J \rightarrow J-2) = \frac{5}{16\pi} e^2 |\langle JK20 | J-2, K \rangle|^2 Q_0(t)^2 \quad K \neq 1/2, 1;$$

Elliott's Model

The expression for the quadrupole moments is also valid in the Elliott's model. However the one for the $B(E2)$'s is only approximately valid for very low spins. Using them it can be easily verified that the $SU(3)$ predictions compare nicely with the experimental results

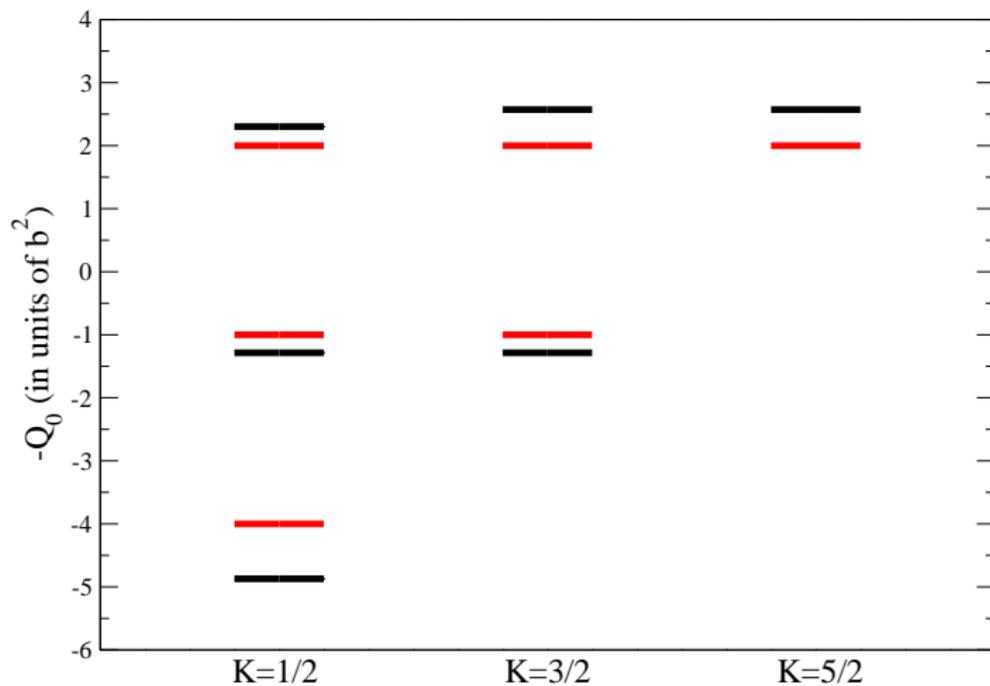
$$Q_{spec}(2^+) = -23(3) \text{ efm}^2 \text{ and } B(E2)(2^+ \rightarrow 0^+) = 66(3) \text{ e}^2\text{fm}^4 \text{ for } {}^{20}\text{Ne}$$

$$Q_{spec}(2^+) = -17(1) \text{ efm}^2 \text{ and } B(E2)(2^+ \rightarrow 0^+) = 70(3) \text{ e}^2\text{fm}^4 \text{ for } {}^{24}\text{Mg}$$

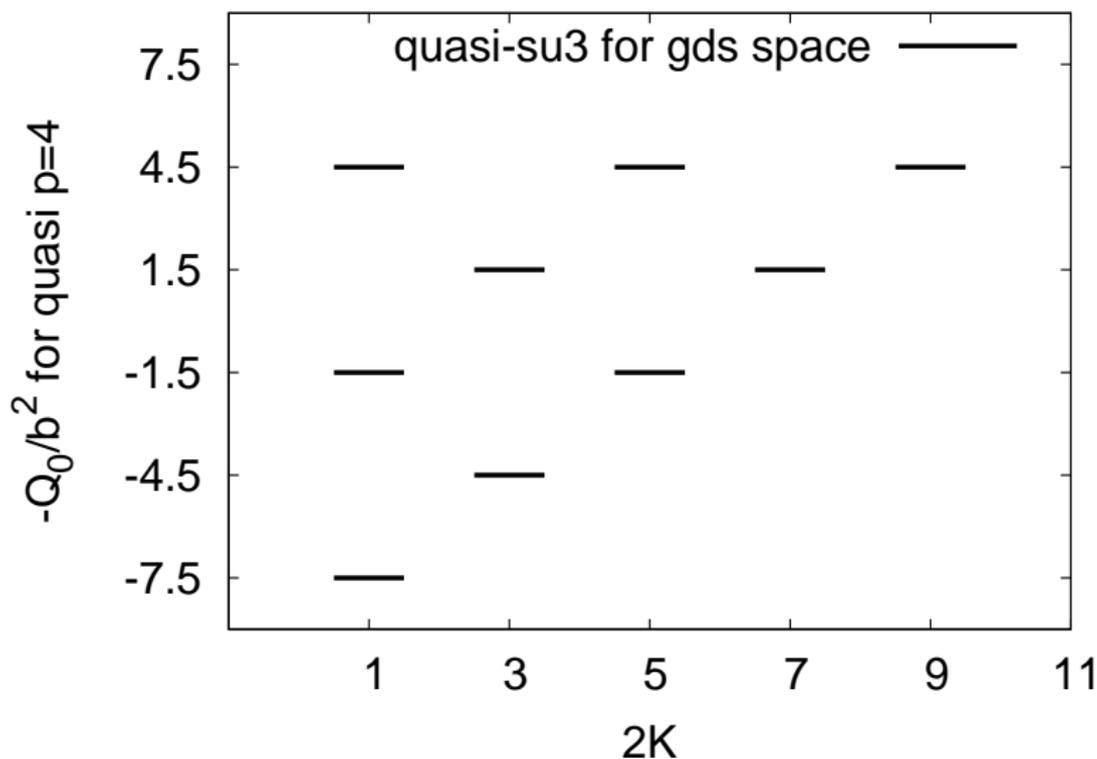
SU3 variants, Pseudo and Quasi-SU3

Besides Elliott's SU(3) there are other approximate symmetries related to the quadrupole quadrupole interaction which are of great interest. Pseudo-SU3 applies when the valence space consists of a quasi-degenerate harmonic oscillator shell except for the orbit with maximum j , we had denoted this space by r_ρ before. Its quadrupole properties are close to those of SU(3) in the shell with $(p-1)$. Quasi-SU3 applies in a regime of large spin orbit splitting, when the valence space contains the intruder orbit and the $\Delta j=2, \Delta l=2$; $\Delta j=4, \Delta l=4$; etc, orbits obtained from it. Its quadrupole properties are similar to those of SU3 as well.

Pseudo-SU3 intrinsic states



Quasi-SU3 intrinsic states



The quadrupole interaction in a single orbit

The intrinsic quadrupole moment for n particles in an orbit j with principal HO quantum number p is given by the formula:

$$\frac{Q_0}{b^2} = \sum_m 2r^2 \langle jm | C_2 | jm \rangle = \sum_m (p + 3/2) \frac{j(j+1) - 3m^2}{j(j+1)}$$

If we fill orderly the magnetic sub-states with increasing $|m|$ we obtain prolate intrinsic states. If we do it the other way around, we obtain oblate intrinsic states.

The quadrupole interaction in a single orbit

In the table, we list the Q_0 values for the $0g_{9/2}$ orbit and $N=Z$ (in units of b^2). For $n < (2j+1)$ the oblate solutions have the larger Q_0 (and therefore the larger binding if the quadrupole interaction is dominant). For $n > (2j+1)$ the prolate solutions lead. For $n = (2j+1)$ both are degenerate.

n	2	4	6	8	10	12	14	16	18
prol	5.3	10.7	14.7	18.7	20	21.3	18.7	16	8
-obl	8	16	18.7	21.3	20	18.7	14.7	10.7	5.3

Their role far from stability

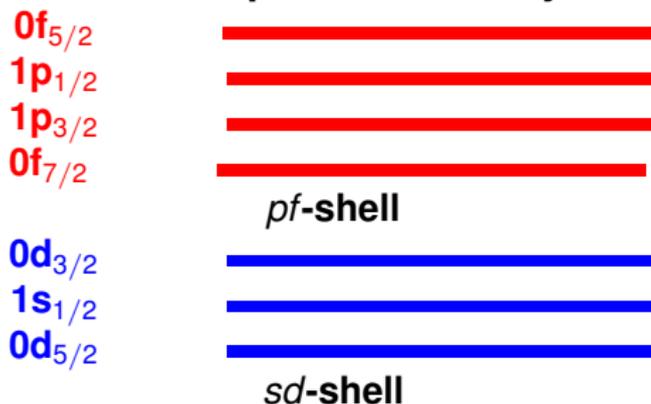
These symmetries turn out to be at the root of the appearance of islands of inversion far from stability. They are more prominent at the neutron rich side and occur when the configurations which correspond to the neutron shell closures at $N=8, 20, 28$ and 40 are less bound than the intruder ones (more often deformed) built by promoting neutrons across the Fermi level gap.

Their role far from stability

The reason of the inversion is that the intruder configurations maximize the quadrupole correlations and thus their energy gains. This is only possible when the orbits around the Fermi level can develop the symmetries of the quadrupole interaction. For instance, at $N=20$ the intruder states in ^{32}Mg have four sd protons in Quasi-SU3, two sd neutron holes in Pseudo-SU3 and two pf neutrons in Quasi-SU3. This leads to a huge gain of correlation energy (typically 12 MeV) which suffices to turn the intruders into ground states.

Coexistence: Spherical, Deformed and Superdeformed states in ^{40}Ca . A full SM-CI calculation

In the valence space of two major shells



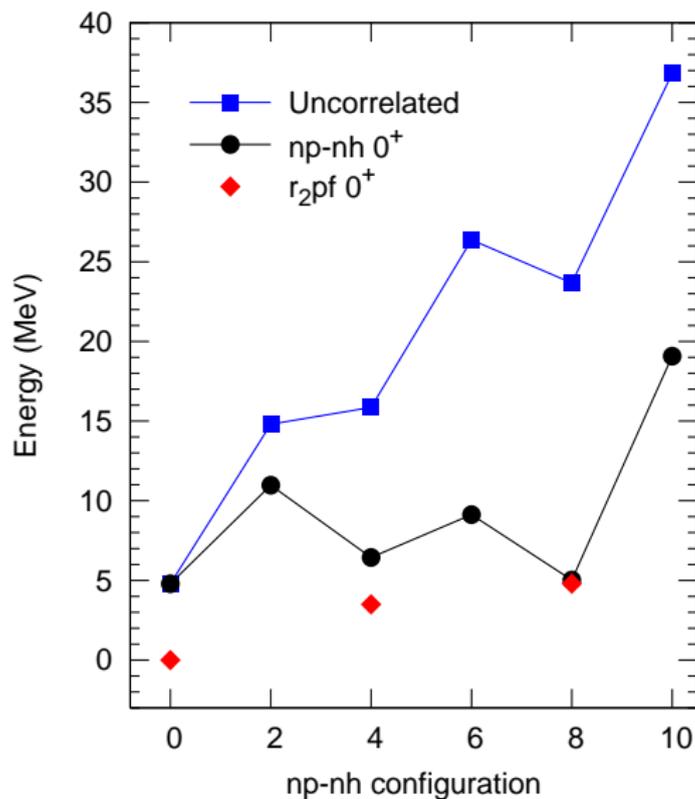
The relevant configurations are:

$[sd]^{24} 0p-0h$ in ^{40}Ca , SPHERICAL

$[sd]^{20} [pf]^4 4p-4h$ in ^{40}Ca , DEFORMED

$[sd]^{16} [pf]^8 8p-8h$ in ^{40}Ca , SUPERDEFORMED

The correlation energies



The correlation energies

- In the 8p-8h configuration the correlations amount to 18.5 MeV. 5.5 MeV are due to T=1 pairing and 0.5 MeV to T=0 pairing, thus the neutron-proton pairing contribution is 2.33 MeV. The remaining 12.5 MeV are most likely of quadrupole origin.
- In the 4p-4h configuration, the correlation energy is about one half of this.
- The physical ground state gains 5 MeV of pairing energy by mixing with the other np-nh states, the ND bandhead 2 MeV, and the SD bandhead nothing
- The dimension of the basis in the full SM-CI calculation is 10^9 . The present limit of basis size in our calculations is 2.5×10^{10} M=0 Slater determinants

SU(3) predictions

In the 4p-4h intrinsic state of ^{40}Ca , the two neutrons and two protons in the pf -shell can be placed in the lowest $K=1/2$ quasi-SU3 level of the $p=3$ shell. This gives a contribution $Q_0=25 \text{ b}^2$. In the pseudo-sd shell, $p=1$ we are left with eight particles, that contribute with $Q_0=7 \text{ b}^2$. In the 8p-8h the values are $Q_0=35 \text{ b}^2$ and $Q_0=11 \text{ b}^2$

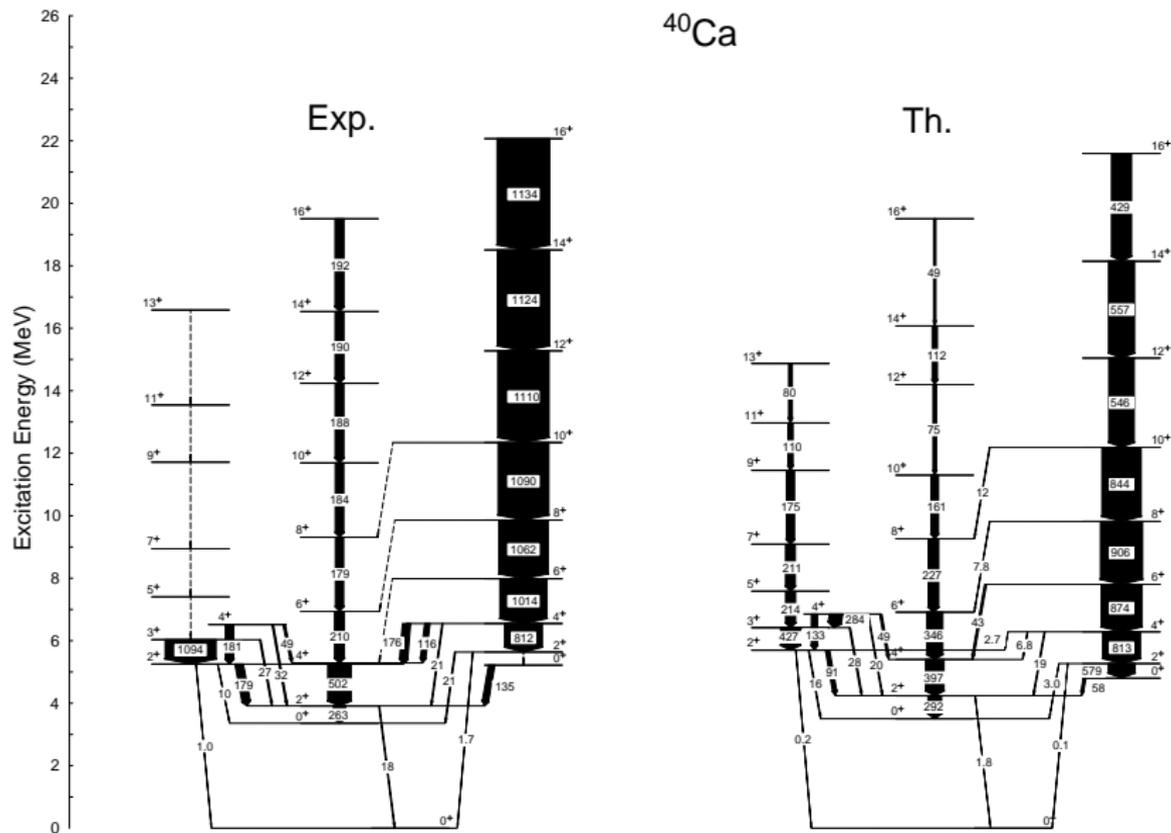
Using the proper values of the oscillator length it obtains:

^{40}Ca 4p-4h band $Q_0=125 \text{ e fm}^2$ ($Q_0=148 \text{ e fm}^2$)

^{40}Ca 8p-8h band $Q_0=180 \text{ e fm}^2$ ($Q_0=226 \text{ e fm}^2$)

In very good accord with the data ($Q_0=120 \text{ e fm}^2$ and $Q_0=180 \text{ e fm}^2$). The values in blue assume strict SU3 symmetry in both shells. The SM results almost saturate the quasi-SU3 bounds. The SU3 values are a 25% larger.

Comparing with experiment

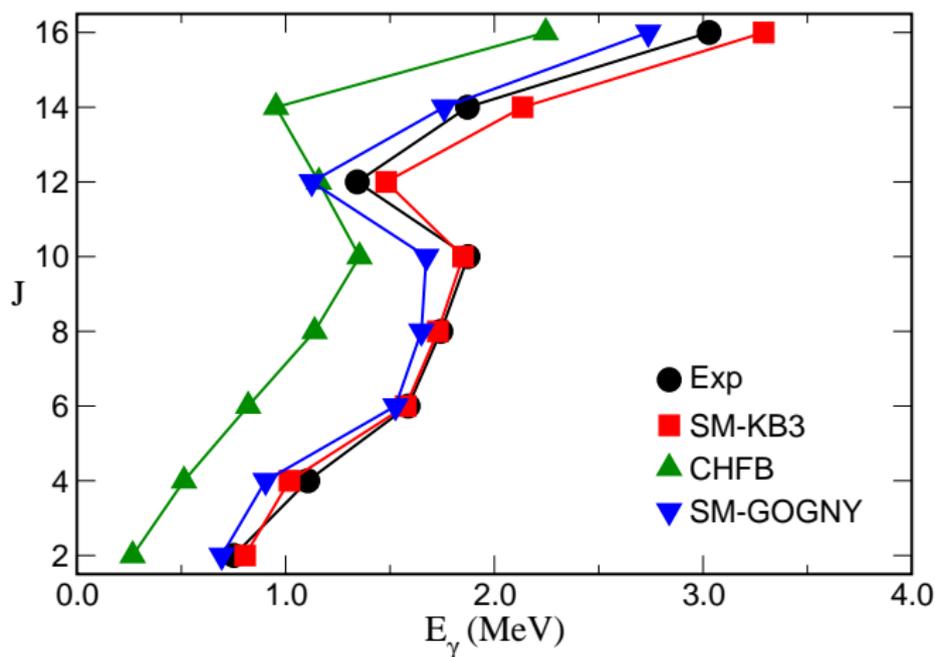


Deformed nuclei; Intrinsic vs. Laboratory Frame Approaches

A case where the two approaches could be confronted was ^{48}Cr (four protons and four neutrons on top of ^{40}Ca suffice to produce a well behaved rotor) where an ISM description in the full pf -shell was for the first time possible a few lustra ago.

The mean field intrinsic description was a Cranked Hartree Fock Bogolyuvov description using the Gogny force. Both calculations reproduce the rotor like behavior at low and medium spin and the backbending at $J=12$. However, the CHFB description misses badly the size of the moment of inertia due to absence of neutron proton pairing correlations in its wave functions. The Gogny force does contain the right proton neutron $T=0$ and $T=1$ pairing as shown by the results of the ISM calculation with its two body matrix elements.

ISM dialogues with CHFB



From the laboratory to the intrinsic frame

The transformation rules from the laboratory to the intrinsic frame quantities and vice versa can be written, in the Bohr Mottelson model as:

$$Q_0(s) = \frac{(J+1)(2J+3)}{3K^2 - J(J+1)} Q_{spec}(J), \quad K \neq 1$$

$$B(E2, J \rightarrow J-2) = \frac{5}{16\pi} e^2 |\langle JK20 | J-2, K \rangle|^2 Q_0(t)^2 \quad K \neq 1/2, 1;$$

To have a good deformed rotor, the Q's and the B(2)'s in the laboratory frame must be consistent with a common value of the intrinsic quadrupole moment

ISM dialogues with CHFB

The laboratory frame wave-functions are indeed collective as can be seen in this table. From the calculated values we can extract the intrinsic quadrupole moments which are roughly independent of J below the backbending as in a well behaved Bohr-Mottelson rotor. From the intrinsic quadrupole moment we extract a deformation parameter $\beta=0.28$ which is in very good agreement with the CHFB result.

J	$B(E2)_{exp}$	$B(E2)_{th}$	$Q_0(B(E2))$
2	321(41)	228	107
4	330(100)	312	105
6	300(80)	311	100
8	220(60)	285	93
10	185(40)	201	77
12	170(25)	146	65
14	100(16)	115	55
16	37(6)	60	40

The intrinsic state in the CHFB description

