Theoretical Nuclear Structure: A Primer

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ABSTRACT

In these lecture notes I will review the basic elements of the nuclear many body problem. After a discussion of the Independent Particle Model I will introduce the nuclear effective interaction in its Fock space representation. I will then separate its Monopole and Multipole terms and discuss the dominant terms of the Multipole hamiltonian; the drivers of the very strong nuclear correlations. I will then describe microscopically the most important manifestations of these correlations in the nucleus: the superfluidity governed by the pairing interaction; the nuclear vibrations, mainly of quadrupole and octupole type and the definition of the nuclear phonons, and finally I will address the microscopic description of the permanently deformed nuclear rotors in the laboratory frame, a shape transition provoked by the quadrupole quadrupole interaction.

CONTENTS

I. INTRODUCTION TO THE NUCLEAR MANY-BODY PROBLEM

In the Standard Model of Nuclear Structure the elementary components are nucleons (N neutrons and Z protons, N+Z=A). The mesonic and quark degrees of freedom are integrated out. In most cases non-relativistic kinematics is used. The bare nucleon-nucleon (or nucleon-nucleon-nucleon) interactions are inspired by meson exchange theories or more recently by chiral perturbation theory, and must reproduce the nucleon-nucleon phase shifts, and the properties of the deuteron and other few body systems. The challenge is to find $\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \ldots \vec{r}_A)$ such that HΨ=EΨ, with:

$$H = \sum_{i}^{A} T_i + \sum_{i,j}^{A} V_{2b}(\vec{r}_i, \vec{r}_j) + \sum_{i,j,k}^{A} V_{3b}(\vec{r}_i, \vec{r}_j, \vec{r}_k) \tag{1}$$

The knowledge of the eigenvectors Ψ and the eigenvalues E make it possible to obtain electromagnetic moments, transition rates, weak decays, cross sections, spectroscopic factors, etc. The task is indeed formidable. Only very recently and only for very light nuclei A$\leq$10 the problem has been solved "exactly" thanks to the pioneer work of Pandharipande, Wiringa and Pieper, [1] which used variational methods (Green Function) solved by Monte Carlo techniques (GFMC). More recently, the perturbative approach has been implemented in the framework of the No Core Shell Model (NCSM) by Barrett, Navratil, and Vary [2]. And even more recently, the techniques of lattice gauge theory together with Chiral Perturbation Theory have been used with very promising results in very light nuclei [3]

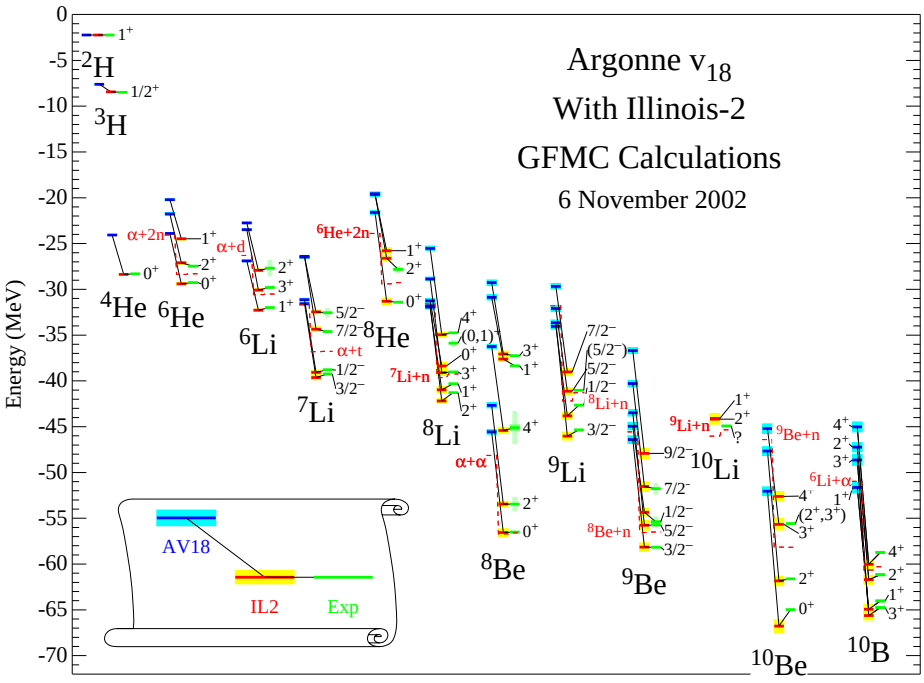


FIG. 1. (color online) Comparison of the GFMC results with the experimental data with and without three body forces

A very important outcome of these calculations is the compulsory need to include three body forces in order to get correct solutions of the nuclear many body problem. The GFMC and the NCSM are severely limited by the huge size of the calculations when A becomes larger

than twelve. For the rest of the chart of nuclides, approximate methods have to be used. Except for the semiclasical ones (liquid drop) and the α-cluster models, all are based on the Independent Particle Approximation. Beyond the limits of applicability of the fully "ab initio" descriptions, the methods of choice are the Interacting Shell Model (noted ISM or SM-CI) and the Mean Field (and Beyond) approaches using Energy Density Functionals (aka density dependent effective interactions, like the Gogny force). There is nowadays renewed efforts to connect rigorously these two global methods and the bare two and three body nuclear interactions by means of the full palette of the Many Body Perturbation Methods. If this is achieved, they will deserve also the "ab initio" label.

II. THE INDEPENDENT PARTICLE MODEL

The basic idea of the Independent Particle Mode (IPM) is to assume that, at zeroth order, the result of the complicated two body interactions among the nucleons is to produce an average self-binding potential. Mayer and Jensen (1949) proposed an spherical mean field consisting in an isotropic harmonic oscillator plus a strongly attractive spin-orbit potential and an orbit-orbit term.

$$H = \sum_i h(\vec{r}_i) \tag{2}$$

$$h(r) = -V_0 + t + \frac{1}{2}m\omega^2 r^2 - V_{so}\vec{l}\cdot\vec{s} - V_B l^2 \tag{3}$$

Later, other functional forms which follow better the form of the nuclear density and have a more realistic asymptotic behavior, *e.g.* the Woods-Saxon well, were adopted

$$V(r) = V_0\left(1 + e^{\frac{r-R}{a}}\right)^{-1} \tag{4}$$

with

$$V_0 = \left(-51 + 33\frac{N-Z}{A}\right) MeV \tag{5}$$

and

$$V_{ls}(r) = \frac{V_0^{ls}}{V_0}(\vec{l}\cdot\vec{s})\frac{r_0^2}{r}\frac{dV(r)}{dr}\ ;\ V_0^{ls} = -0.44V_0 \tag{6}$$

The eigenvectors of the IPM are characterized by the radial quantum number n, the orbital angular momentum l, the total angular momentum j and its Z projection m. With the choice of the harmonic oscillator, the eigenvalues are:

$$\epsilon_{nljm} = -V_0 + \hbar\omega(2n + l + 3/2)$$

$$-V_{so}\frac{\hbar^2}{2}(j(j+1) - l(l+1) - 3/4) - V_B\hbar^2 l(l+1) \tag{7}$$

In order to reproduce the nuclear radii,

$$\hbar\omega = 45A^{-1/3} - 25A^{-2/3} \tag{8}$$

With a suitable choice of the parameters, it explains the magic numbers and, in the large A limit, the volume, the surface and (half) the symmetry terms of the semi-empirical mass formula as well (more on that later).

The wave functions of the isotropic harmonic oscillator without spin-orbit can be written as:

$$\Psi_{nlm}(r,\theta,\phi) = \frac{1}{r}\, R_{nl}(r)\, Y_{lm}(\theta,\phi) \tag{9}$$

By convention the n's start at zero, therefore the self energies read:

$$E_{nl} = (2n + l + 3/2)\, \hbar\omega = (p + 3/2)\hbar\omega \tag{10}$$

$Y_{lm}(\theta,\phi)$ are the spherical harmonics and:

$$R_{nl}(r) = (-1)^l \left(\frac{2\,(2\nu)^{l+3/2}\, n!}{\Gamma(n + l + 3/2)}\right)^{1/2} r^{l+1}\, e^{-\nu r^2}\, L_n^{l+1/2}(2\nu r^2) \tag{11}$$

The parameter ν is defined as $\dfrac{m\omega}{2\hbar}$, thus $2\nu = \dfrac{1}{b^2}$. The degeneracy of each shell is (p+1)(p+2), and the L's are the Laguerre (associated) polynomials, defined as:

$$L_k^r(x) = (-1)^k \sum_{p=0}^{k} (-1)^p\, \frac{\Gamma(r + k + 1)}{p!\,(k - p)!\,\Gamma(r + k - p + 1)}\, x^{k-p} \tag{12}$$

k takes the values 0, 1, 2, ... The Γ functions are defined by:

$$\Gamma(a) = \int_0^\infty x^{a-1}\, e^{-x}\, dx \tag{13}$$

and verify $\Gamma(a + 1) = a\,\Gamma(a)$. When the spin orbit coupling is taken into account, we must include explicitly the spin part of the wave function and change the coupling scheme from [**L S**] to [**JJ**].

- VOCABULARY
  - STATE: a solution of the Schrödinger equation with a one body potential; e.g. the H.O. or the W.S. It is characterized by the quantum numbers $nljm$ and the projection of the isospin t_z
  - ORBIT: the ensemble of states with the same nlj, e.g. the 0d5/2 orbit. Its degeneracy is (2j+1)
  - SHELL: an ensemble of orbits quasi-degenerated in energy, e.g. the pf shell
  - MAGIC NUMBERS: the numbers of protons or neutrons that fill orderly a certain number of shells
  - GAP: the energy difference between two shells
  - SPE, single particle energies, the eigenvalues of the IPM hamiltonian
  - ESPE, effective single particle energies, the eigenvalues of the monopole hamiltonian.

III. THE INDEPENDENT PARTICLE MODEL AND THE LIQUID DROP MASS FORMULA

The IPM explains the magic numbers, the spins and parities of the ground states and some excited states of doubly magic nuclei plus or minus one nucleon, their magnetic moments, etc. With the addition of an schematic pairing tern between like particles it can go a bit further in semi-magic nuclei (Schmidt lines). What is less well known is that in the large A limit, the IPM can reproduce the volume, the surface and the symmetry terms of the semi-empirical mass formula as well.

Let's take the IPM with an HO potential and neglect the spin orbit term. Then:

$$H = \sum_i t_i - V_0 + \frac{1}{2} m\omega^2 r_i^2$$

The single particle energies are: $\epsilon_i = -V_0 + \hbar\omega(p_i + 3/2)$ and $< r_i^2 >= b^2(p_i + 3/2)$ with $b^2 = \dfrac{\hbar}{m\omega}$. The degeneracy of each shell is d=(p+1)(p+2) for protons and for neutrons. Assuming N=Z, to accommodate A/2 identical particles we need to fill the shells up to p=p$_F$. Experimentally, the radius of the nucleus is given by $< r^2 >= \frac{3}{5}R^2 = \frac{3}{5}(1.2A^{1/3})^2$, and in the IPM by:

$$< r^2 >= \frac{2}{A}\sum_i^{A/2} < r_i^2 >= \frac{2}{A}\sum_{p=0}^{p_F} b^2(p + 3/2)(p + 1)(p + 2)$$

From

$$\frac{A}{2} = \sum^{p_F}(p + 1)(p + 2)$$

it obtains at leading order, $p_F = (\frac{3}{2}A)^{3/2}$. Putting everything together we find, at leading order in p_F, $b^2 = A^{1/3}$ and $\hbar\omega = 41 \cdot A^{-1/3}$. We can now compute the total binding energy as:

$$B = \sum_{i=1}^{A}(-V_0 + \hbar\omega(p_i + 3/2))$$

that gives at leading order:

$$\frac{B}{A} + V_0 = \hbar\omega \cdot \frac{p_F^4}{4} \cdot \frac{2}{A} = \hbar\omega\left(\frac{3A}{2}\right)^{4/3}\frac{1}{2A} = \hbar\omega A^{1/3}\frac{1}{2}\left(\frac{3}{2}\right)^{4/3}$$

Finally we have

$$\frac{B}{A} = -V_0 + 41 \times 0.86$$

and we recover the volume term of the semi empirical mass formula for $V_0 \sim 50$ MeV.

If we go to next to leading order, keeping the terms in p_F^3, we recover the surface term with the correct coefficient . We can repeat the calculation at leading order but with N≠Z, and obtain:

$$B = -AV_0 + \frac{\hbar\omega}{4}((p_F^\nu)^4 + (p_F^\pi)^4) = -AV_0 + \frac{\hbar\omega}{4}((3N)^{4/3} + (3Z)^{4/3})$$

Making a Taylor expansion around the minimum at N=Z and using the previously determined values we find an extra term of the form (N-Z)^2/A with a coefficient which does not agree with the one resulting from the fit of the semi empirical mass formula to the experimental binding energies (a_{sym} = 23 MeV). This reflects the fact that the nuclear two body neutron-proton interaction is in average more attractive than the neutron-neutron and the proton proton ones, and it is related as well to the experimental evidence of the near equality of the neutron and proton radii for N≠Z . Therefore we should use different values of $\hbar\omega$ and V_0's for protons and neutrons in the derivation, which complicates a lot the calculation because both effects go in opposite directions.

IV. THE MEANING OF THE INDEPENDENT PARTICLE MODEL

The usual procedure to generate a mean field in a system of N interacting fermions, starting from their free interaction, is the Hartree-Fock approximation, extremely successful in atomic physics. Whatever the origin of the mean field, the eigenstates of the N-body problem are Slater determinants *i.e.* anti-symmetrized products of N single particle wave functions. In the nucleus, there is a catch, because the very strong short range repulsion and the tensor force make the HF approximation based upon the bare nucleon-nucleon force impracticable. However, at low energy, the nucleus do manifest itself as a system of independent particles in many cases, and when it does not, it is due to the medium range correlations that produce strong configuration mixing and not to the short range repulsion. Does the success of the shell model really "prove" that nucleons move independently in a fully occupied Fermi sea as assumed in HF approaches? In fact, the single particle motion can persist at low energies in fermion systems due to the suppression of collisions by Pauli exclusion (see Pandharipande et al., [4]) Brueckner theory takes advantage of the Pauli blocking to regularize the bare nucleon- nucleon interaction, in the form of density dependent effective interactions of use in HF calculations or G-matrices for large scale shell model calculations.

An example of regularized interaction is the one proposed by Brink and Boeker [5], whose central part is:

$$V_c(|\vec{r}_1 - \vec{r}_2|) = \sum_{i=1}^{2}[1 - m_i(1 + P_\sigma P_\tau)]\; v_i\; e^{-|\vec{r}_1 - \vec{r}_2|^2/\mu_i^2} \tag{14}$$

For the spin orbit they took a one body approximation:

$$V_{ls} = \frac{-12 \text{ MeV}}{\hbar^2\sqrt{A}}\; \vec{l}\cdot\vec{s} \tag{15}$$

The values of the parameters are:

i	μ_i(fm)	v_i (MeV)	m_i
1	0.7	471.1	-0.43
2	1.4	-163.8	0.51

To be more realistic, one should refine the channel dependence of the central terms, include a two body spin-orbit interaction, and more importantly, a term which depends on the density.

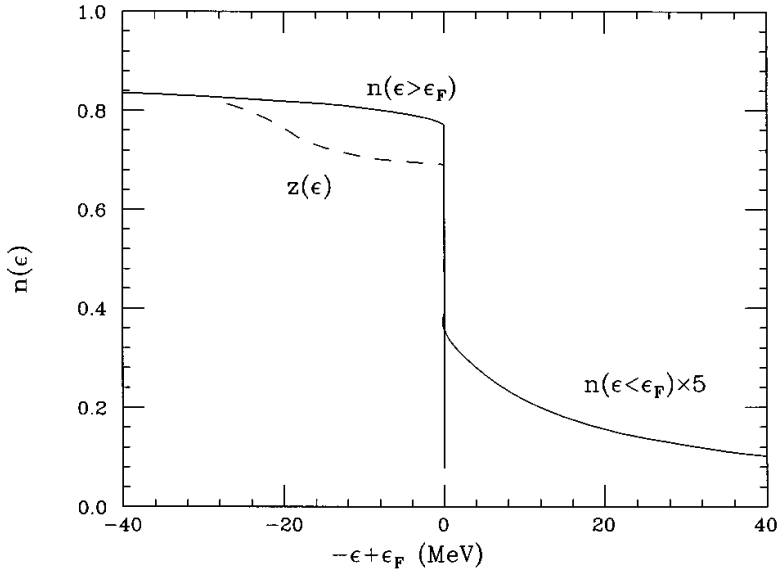


FIG. 2. Dilution of the Spectroscopic strength by the bare N-N interaction. Results for nuclear matter.

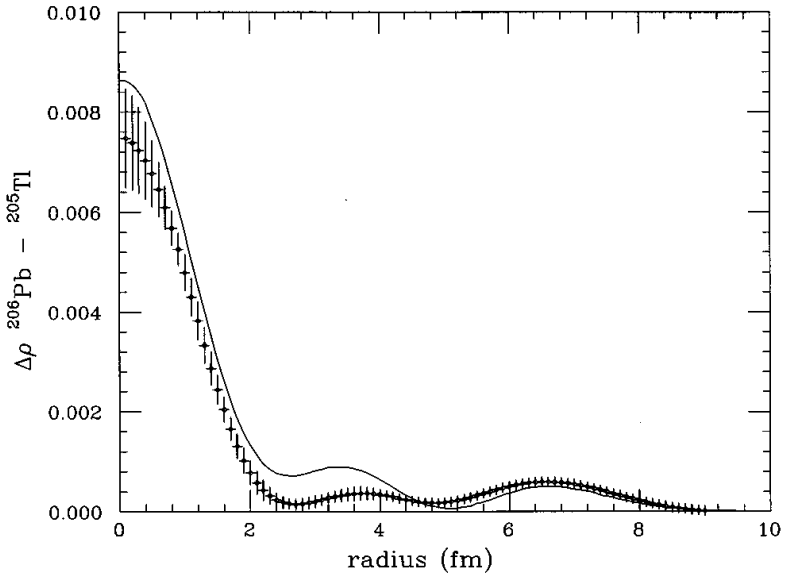


FIG. 3. The charge density difference between ^{206}Pb and ^{205}Tl, experiment compared with the IPM description

After this re-vamping, the Brink and Boeker interaction becomes the Gogny interaction [6] extremely successful in numerous mean field applications (and beyond).

The wave function of the ground state of a nucleus in the IPM is the product of a Slater determinant for the Z protons that occupy the Z lowest states in the mean field and another Slater determinant for the N neutrons in the N lowest states of the mean field. In second quantization, this state can be written as:

$$|N\rangle \cdot |Z\rangle \tag{16}$$

with

$$|N\rangle = n_1^\dagger n_2^\dagger \dots n_N^\dagger |0\rangle \tag{17}$$

$$|Z\rangle = z_1^\dagger z_2^\dagger \dots z_Z^\dagger |0\rangle \tag{18}$$

In a system of non interacting fermions the occupied states have occupation number 1 and the empty ones occupation number 0. In reality we find rather the situation depicted in Figure 2. In spite of that, the nuclear quasi-particles resemble extraordinarily to the mean field solutions of the IPM. This was demonstrated by the beautiful electron scattering experiment of Cavedon *et al.*(1982) [7] in which they extracted the charge density difference between ^{206}Pb and ^{205}Tl, that, in the IPM limit is just the square of the $2s_{1/2}$ orbit wave function.

As can be seen in Figure 3, the shape of the $2s_{1/2}$ orbit is very well given by the mean field calculation. To make the agreement quantitative the calculated density had to be scaled down with the occupation number. This is a first example of the necessity of using effective transition operators consistent with the regularized interactions that provide the natural basis for the many body description of nuclei. For a very pedagogical discussion of the basis of the IPM, read the article " Independent particle motion and correlations in fermion systems" by V. R. Pandharipande, et al., RMP 69 (1997) 981.

V. BEYOND THE INDEPENDENT PARTICLE MODEL

It is quite obvious that the IPM cannot encompas the extreme variety of manifestations of the nuclear dynamics. In fact, even in the most favorable cases, as at the doubly magic nuclei, its limitations are dramatically evident. Just a look at Figure 4 proves it. There we have plotted part of the level scheme of ^{40}Ca. In the IPM limit we expect a 0^+ ground state (no problem) and a gap of about $\hbar\omega$ (10 MeV) before finding a bunch of quasi-degenerate levels of particle-hole type and negative parity. In fact, the first excited state lies at 3.5 MeV and is again a 0^+, which, upon experimental and theoretical scrutiny turns out to be the band head of a deformed band of 4p-4h nature. Even more exotic is the 0^+ at 5.1 MeV, which is the band head of a superderformed! band of 8p-8h structure. Going beyond the mean field is compulsory because the nuclear dynamics is dominated in most cases by the correlations. We shall show at the end of these notes how these coexisting structures can be reproduced by large scale shell model interactions and interpreted using analytic models
To go beyond the IPM, there are two main routes; The mean field way relies in Hartree Fock based approaches which use density dependent interactions of different sort; Skyrme, Gogny, or Relativistic Mean Field parametrizations. The correlations are taken into account by explicitly breaking the symmetries in the mean field. That's why they are often referred to as "intrinsic" descriptions. Projections before (VAP) or after (PAV) variation are enforced to restore the conserved quantum numbers. Ideally, configuration mixing is also implemented through the Generator Coordinate Method. The other route pertains to the Interacting Shell Model (ISM) which can be seen as an approximation to the exact solution of the nuclear A-body problem using effective interactions in restricted spaces. The ISM wave functions respect the symmetries of the Hamiltonian and these approaches are sometimes called "laboratory frame" descriptions.

Let's proceed through a kind of formal solution to the A-body problem. The single particle states (i,j, k, ...), which are the solutions of the IPM, provide as well a basis in the

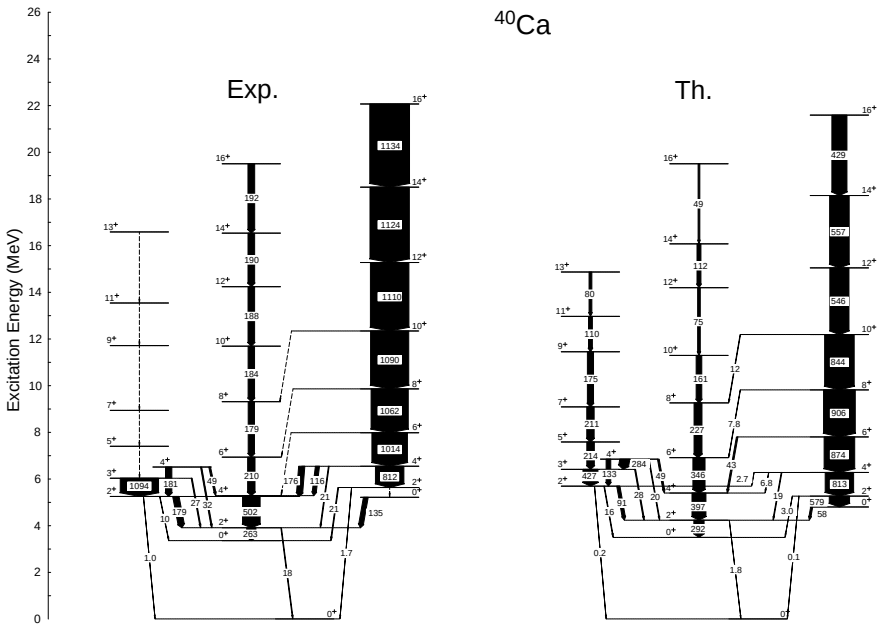


FIG. 4. Partial level scheme of ^{40}Ca; experiment vs large scale shell model results [8]

space of the occupation numbers (Fock space). The many body wave functions are Slater determinants:

$$\Phi = a^\dagger_{i_1}, a^\dagger_{i_2}, a^\dagger_{i_3}, \ldots a^\dagger_{i_A}|0\rangle \tag{19}$$

We can distribute the A particles in all the possible ways in the available single particle states. This provides a complete basis in the Fock space. The number of Slater determinants will be huge but not infinite because the theory is no longer valid beyond a certain cutt-off. Therefore, the "exact" solution can be expressed as a linear combination of the basis states:

$$\Psi = \sum_\alpha c_\alpha \Phi_\alpha \tag{20}$$

and the solution of the many body Schödinger equation

$$H\Psi = E\Psi \tag{21}$$

is transformed in the diagonalization of the matrix:

$$\langle \Phi_\alpha | H | \Phi_\beta \rangle \tag{22}$$

whose eigenvalues and eigenvectors provide the "physical" energies and wave functions. A Shell Model calculation thus amounts to diagonalizing the effective nuclear hamiltonian in the basis of all the Slater determinants that can be built distributing the valence particles in a set of orbits which is called "valence space". The orbits that are always full form the "core". If we could include all the orbits in the valence space (a full No Core calculation) we should get the "exact" solution. The effective interactions are obtained from the bare nucleon-nucleon interaction by means of a regularization procedure aimed to soften the short range repulsion. In other words, using effective interactions we can treat the A-nucleon system in a basis of independent quasi-particles. As we reduce the valence space, the interaction has to be renormalized again using Many Body Perturbation Theory. The three pillars of the shell model are then the effective interactions, the valence spaces and

the algorithms and codes put at work to solve the huge computational challenges posed by the solution of this secular problem. See for instance, E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves and A. P. Zuker. "The Shell Model as a Unified View of Nuclear Structure", Reviews of Modern Physics, 77 (2005) 427. The effective interactions for CI (configuration interaction)-SM calculations are obtained from the bare nucleon-nucleon interaction by means of a regularization procedure aimed to soften the short range repulsion. In other words, using effective interactions we can treat the A-nucleon system in a basis of independent quasi-particles. As we reduce the valence space, the interaction has to be renormalized again in a perturbative way. Up to this point these calculations are in fact "ab initio" In fact, the realistic NN interactions seem to be correct except for its simplest part, the monopole hamiltonian responsible for the evolution of the spherical mean field. Therefore, we surmise that the three body forces will mainly contribute to the monopole hamiltonian.

VI. THE EFFECTIVE INTERACTIONS IN FOCK'S SPACE

Using the creation and annihilation operators of particles in the states of the underlying spherical mean field in the coupled representation, we can write the Hamiltonian as:

$$\mathcal{H} = \sum_{rr'} \epsilon_{rr'} (a_r^+ a_{r'})^0 + \sum_{r\leq s, t\leq u, \Gamma} W^{\Gamma}_{rstu} Z^+_{rs\Gamma} \cdot Z_{tu\Gamma}, \tag{23}$$

where Z^+_Γ (Z_Γ) is the coupled product of two creation (annihilation) operators.

$$Z^+_{rs\Gamma} = [a^\dagger_r a^\dagger_s]^\Gamma \tag{24}$$

Γ is a shorthand for (J,T); r, s ..... run over the orbits of the valence space; $\epsilon_{rr'}$ are the single particle energies (or the kinetic energies in the no-core calculations) and W^Γ_{rstu} the antisymmetrized two body matrix elements:

$$W^\Gamma_{rstu} = \langle j_r j_s (JT) | V | j_t j_u (JT) \rangle \tag{25}$$

In the occupation number representation (Fock space) all the information about the interaction is contained in its two body matrix elements. The many body problem then reduces to the manipulation of the creation and annihilation operators using the Wick theorem and techniques alike.
The most general method to compute the two body matrix elements is due to Slater and carries its name. When the independent particle wave functions are those of the harmonic oscillator or if they can be represented by linear combination of a few harmonic oscillator states, the method of choice is that of Brody and Moshinsky.

A. Slater's method

For a general central interaction, the two body matrix elements involve integrals in the coordinates of the two particles, $\vec{r}_1$ and $\vec{r}_2$ of a product of functions of $\vec{r}_1$ and $\vec{r}_2$ (the IPM wave functions) and a function of $|\vec{r}_1 - \vec{r}_2|$ (the potential) which are not at all straightforward. Slater's method consists in expanding the interaction in a complete set of angular functions, the Legendre polynomials:

$$V(|\vec{r}_1 - \vec{r}_2|) = \sum_{k=0}^{\infty} v_k(r_1, r_2) P_k(cos\ \theta_{12}) \tag{26}$$

$$P_k(cos\ \theta_{12}) = \sum_{\kappa} \frac{4\pi}{(2k+1)} Y_k^{\kappa^*}(\Omega_1) Y_k^{\kappa}(\Omega_2) \tag{27}$$

Let's develop the case of a diagonal matrix element, normalized and anti-symmetrized without isospin for the time being,

$$\langle j_1 j_2(JM)|V_{12}|j_1 j_2(JM)\rangle = \left(\frac{1}{1+\delta_{j_1 j_2}}\right)(\langle j_1 j_2(JM)|V_{12}|j_1 j_2(JM)\rangle_{dir}$$
$$-(-1)^{(j_1+j_2-J)}\langle j_1 j_2(JM)|V_{12}|j_2 j_1(JM)\rangle_{exch}) \tag{28}$$

where we have separated the direct and the exchange term. We can write the direct term as:

$$\langle j_1 j_2(JM)|V_{12}|j_1 j_2(JM)\rangle_{dir} = \sum_k f_k\ F_k \tag{29}$$

$$f_k = \frac{4\pi}{(2k+1)}\langle j_1 j_2(JM)|\mathbf{Y}_k(\Omega_1)\cdot\mathbf{Y}_k(\Omega_2)|j_1 j_2(JM)\rangle \tag{30}$$

$$F_k = \int |u_{n_1 l_1}(r_1) u_{n_2 l_2}(r_2)|^2 v_k(r_1, r_2) dr_1\ dr_2 \tag{31}$$

$$f_k = \frac{4\pi}{(2k+1)}(-1)^{j_1+j_2+J} C6j(j_1, j_2, J; j_2, j_1, k)\langle j_1||\mathbf{Y}_k||j_1\rangle\langle j_2||\mathbf{Y}_k||j_2\rangle \tag{32}$$

The exchange term reads:

$$\langle j_1 j_2(JM)|V_{12}|j_2 j_1(JM)\rangle_{exch} = \sum_k g_k\ G_k \tag{33}$$

$$G_k = \int u_{n_1 l_1}(r_1) u_{n_2 l_2}(r_2) u_{n_1 l_1}(r_2) u_{n_2 l_2}(r_1) v_k(r_1, r_2) dr_1\ dr_2 \tag{34}$$

$$g_k = \frac{4\pi}{(2k+1)}(-1)^{1+J} C6j(j_1, j_2, J; j_1, j_2, k)\langle j_1||\mathbf{Y}_k||j_2\rangle\langle j_2||\mathbf{Y}_k||j_1\rangle \tag{35}$$

For the Coulomb potential, $\frac{1}{r_{12}}$, it is easy to find that:

$$v_k(r_1, r_2) = \frac{r_<^k}{r_>^{k+1}} \tag{36}$$

And it is even easier for a delta force $\delta(r_{12})$ whose multipole decomposition is well known

$$\delta(|\vec{r_1} - \vec{r_2}|) = \sum_k \frac{\delta(r_1.r_2)}{r_1 r_2}\frac{2k+1}{4\pi} P_k(cos\ \theta_{12}) \tag{37}$$

thus leading to:

$$v_k(r_1, r_2) = \frac{\delta(r_1.r_2)}{r_1 r_2}\frac{2k+1}{4\pi} \tag{38}$$

B. Two body matrix elements; Moshinsky's transformation

The hamiltonian of two nucleons in an harmonic oscillator potential can be written as:

$$H = \frac{1}{2m}(\vec{p_1}^{\,2} + \vec{p_2}^{\,2}) + \frac{1}{2}m\omega^2(\vec{r_1}^{\,2} + \vec{r_2}^{\,2})$$

Using the transformation $\vec{r}$=$\vec{r_1}$–$\vec{r_2}$; $\vec{R}$=$\frac{1}{2}$($\vec{r_1}$+$\vec{r_2}$), it becomes:

$$H = \frac{1}{m}\vec{p}^{\,2} + \frac{1}{4}m\omega^2\vec{r}^{\,2} + \frac{1}{4m}\vec{P}^{\,2} + m\omega^2\vec{R}^{\,2}$$

Therefore the wave function of the two nucleons can be written in two ways:

$$|n_1l_1m_1\rangle|n_2l_2m_2\rangle \quad \text{and} \quad |nlm\rangle|N\Lambda M_\Lambda\rangle$$

Both provide equivalent basis for the problem, and therefore it is possible to express the states of one basis as a linear combinations of the states of the other. This is the Moshinsky transformation.

$$|n_1l_1, n_2l_2; LM\rangle = \sum_{n,l,N,\Lambda} \langle nl, N\Lambda; L|n_1l_1, n_2l_2; L\rangle|nl, N\Lambda; LM\rangle$$

The coefficients are named after Brody and Moshinsky which tabulated them in a book published by the UNAM in 1960. The second edition published by Gordon and Breach in 1967 is probably the only physics book which is bilingual spanish english.

Now, the two body matrix elements of a central interaction $V(r)$ are easily obtained as:

$$\langle n_1l_1, n_2l_2; LM|V(r)|n_1'l_1', n_2'l_2'; LM\rangle =$$

$$\sum_{n,n',l,N,\Lambda} \langle nl, N\Lambda; L|n_1l_1, n_2l_2; L\rangle\langle n'l, N\Lambda; L|n_1'l_1', n_2'l_2'; L\rangle\langle nl|V(r)|n'l\rangle$$

More general interactions can be easily incorporated with an extra work of angular momentum algebra. For more detail about the Brody Moshinsky method we refer also to Heyde's book "The Nuclear Shell Model" from which we have also borrowed the discussion of the Slater method.

VII. MONOPOLE AND MULTIPOLE COMPONENTS OF THE INTERACTION

Without loosing the simplicity of the Fock space representation, we can recast the two body matrix elements of any effective interaction in a way full of physical insight, following Dufour-Zuker rules [9].

Any effective interaction can be split in two parts:

$$\mathcal{H} = \mathcal{H}_m(monopole) + \mathcal{H}_M(multipole). \tag{39}$$

where $\mathcal{H}_m$ *contains all the terms that are affected by a spherical Hartree-Fock variation, hence it is responsible for the global saturation properties and for the evolution of the spherical single particle energies.*

$$\mathcal{H}_m = \sum \epsilon_i n_i + \sum \left[\frac{1}{(1+\delta_{ij})} a_{ij}\, n_i (n_j - \delta_{ij}) \right.$$
$$\left. + \frac{1}{2} b_{ij} \left(T_i \cdot T_j - \frac{3 n_i}{4} \delta_{ij} \right) \right] + \sum A_{ijk} n_i n_j n_k \tag{40}$$

The coefficients a and b are defined in terms of the centroïds (angular averages):

$$V_{ij}^T = \frac{\sum_J W_{ijij}^{JT}[J]}{\sum_J [J]} \tag{41}$$

as: $a_{ij} = \frac{1}{4}(3V_{ij}^1 + V_{ij}^0)$, $b_{ij} = V_{ij}^1 - V_{ij}^0$, the sums running over Pauli allowed values.

It is easy to verify that the expectation value of the full Hamiltonian in a Slater determinant for closed shells, has the same expression than the Hartree-Fock energy:

$$\langle H \rangle = \sum_i \langle i|T|i\rangle + \sum_{ij} \langle ij|G|ij\rangle \tag{42}$$

where i and j run over the occupied states. If the two body matrix elements are written in coupled formalism and we denote the orbits by $\alpha,\ \beta, \ldots$, the expression reads:

$$\langle H \rangle = \sum_\alpha (2j_\alpha + 1)\langle \alpha|T|\alpha\rangle + \sum_{\alpha \le \beta} \sum_{J,T} (2J+1)(2T+1)\langle j_\alpha j_\beta (JT)|G|j_\alpha j_\beta (JT)\rangle \tag{43}$$

The Monopole Hamiltonian governs the evolution of effective spherical single particle energies with the number of particles in the valence space, schematically:

$$\epsilon_j(\{n_i\}) = \epsilon_j(\{n_i = 0\}) + \sum_i a_{ij} n_i + \sum_{i,k} A_{ijk} n_i n_k \tag{44}$$

It is important to realize that even small defects in the centroids can produce large changes in the relative position of the different configurations due to the appearance of quadratic terms involving the number of particles in the different orbits.

The Multipole Hamiltonian: $\mathcal{H}_M$ can be written in two representations, particle-particle and particle-hole:

$$\mathcal{H}_M = \sum_{r \le s, t \le u, \Gamma} W_{rstu}^\Gamma Z_{rs\Gamma}^+ \cdot Z_{tu\Gamma}, \tag{45}$$

$$\mathcal{H}_M = \sum_{rstu\Gamma} [\gamma]^{1/2} \frac{(1+\delta_{rs})^{1/2}(1+\delta_{tu})^{1/2}}{4} \omega_{rtsu}^\gamma (S_{rt}^\gamma S_{su}^\gamma)^0, \tag{46}$$

where Z_Γ^+ (Z_Γ) is the coupled product of two creation (annihilation) operators and S^γ is the coupled product of one creation and one annihilation operator.

$$Z_{rs\Gamma}^+ = [a_r^\dagger a_s^\dagger]^\Gamma \tag{47}$$

$$S_{rs}^\gamma = [a_r^\dagger a_s]^\gamma \tag{48}$$

The W and ω matrix elements are related by a Racah transformation,

$$\omega^{\gamma}_{rtsu} = \sum_{\Gamma}(-)^{s+t-\gamma-\Gamma} \left\{ \begin{array}{cc} r & s \\ u & t \end{array} \begin{array}{c} \Gamma \\ \gamma \end{array} \right\} W^{\Gamma}_{rstu}[\Gamma], \tag{49}$$

$$W^{\Gamma}_{rstu} = \sum_{\gamma}(-)^{s+t-\gamma-\Gamma} \left\{ \begin{array}{cc} r & s \\ u & t \end{array} \begin{array}{c} \Gamma \\ \gamma \end{array} \right\} \omega^{\gamma}_{rtsu}[\gamma]. \tag{50}$$

The operators $S^{\gamma=0}_{rr}$ are just the number operators for orbits r and $S^{\gamma=0}_{rr'}$ the spherical Hartree-Fock particle hole vertices. Both must have null coefficients if the monopole hamiltonian satisfies Hartree-Fock self-consistency. The operator $Z^{+}_{rr\Gamma=0}$ creates a pair of particle coupled to J=0. The terms $W^{\Gamma}_{rrss}\ Z^{+}_{rr\Gamma=0} \cdot Z_{ss\Gamma=0}$ represent different kinds of pairing hamiltonians. The operators S^{γ}_{rs} are typical vertices of multipolarity γ. For instance, γ=(J=1,L=0,T=1) contains a $(\vec{\sigma}\cdot\vec{\sigma})$ $(\vec{\tau}\cdot\vec{\tau})$ term which is nothing else but the Gamow-Teller component of the nuclear interaction. The terms S^{γ}_{rs} γ=(J=2,T=0) are of quadrupole type r^2Y_2. They are responsible for the existence of deformed nuclei, and they are specially large and attractive when $j_r - j_s$=2 and $l_r - l_s$=2.

A careful analysis of the available realistic effective nucleon-nucleon interactions obtained with different methods, reveals that the multipole hamiltonian is universal and dominated by BCS-like isovector and isoscalar pairing plus quadrupole-quadrupole and octupole-octupole terms of very simple nature ($r^{\lambda}Y_{\lambda}\cdot r^{\lambda}Y_{\lambda}$). As an example we list in Table I the strengths of the coherent multipole components of different interactions for the pf-shell.

TABLE I. Strengths of the coherent multipole components of different interactions for the pf-shell.

Interaction	particle-particle		particle-hole		
	JT=01	JT=10	$\lambda\tau$=20	$\lambda\tau$=40	$\lambda\tau$=11
KB3	-4.75	-4.46	-2.79	-1.39	+2.46
FPD6	-5.06	-5.08	-3.11	-1.67	+3.17
GOGNY	-4.07	-5.74	-3.23	-1.77	+2.46
GXPF1	-4.18	-5.07	-2.92	-1.39	+2.47
BONNC	-4.20	-5.60	-3.33	-1.29	+2.70

VIII. VALENCE SPACES AND CODES

An ideal valence space should incorporate the most relevant degrees of freedom for the nuclei under study and be computationally tractable. Classical $0\hbar\omega$ valence spaces are provided by the major oscillator shells p, sd and pf. As we move far form stability other choices are compulsory; for instance for the very neutron rich nuclei around N=28, a good choice is to take the sd shell for protons and the pf shell for neutrons, for the very neutron rich Cr, Fe, Ni, and Zn, one should rather take r_3-$(0g_{9/2}, 1d_{5/2})$ for the neutrons and pf for protons (in a major harmonic oscillator shell of principal quantum number **p** the orbit j=p+1/2 is called *intruder* and the remaining ones are denoted by r_p). To describe the intruders around N and/or Z=20, a good valence space is r_2-pf. For the nuclei above ^{100}Sn, the valence space r_4-$h_{11/2}$ has been also widely used.

Algorithms include Direct Diagonalisation, Lanczos, Monte Carlo Shell Model, Quantum Monte Carlo Diagonalization, Density Matrix Renormalization Group, etc. There are also a

number of different extrapolation ansatzs. The Strasbourg-Madrid codes (Antoine, Nathan), can deal with problems involving basis of 10^{10} Slater determinants, using relatively modest computational resources. Other competitive codes in the market are OXBACH, NUSHELL and MSHELL.

IX. COLLECTIVITY IN NUCLEI: BASICS

For a given interaction, a many body system would or would not display coherent features at low energy depending on the structure of the mean field around the Fermi level. So, when the spherical mean field around the Fermi surface makes the pairing interaction dominant, the nucleus becomes superfluid, if the quadrupole-quadrupole interaction is dominant the nucleus acquires permanent deformation, and in the extreme limit in which the monopole hamiltonian would be negligible, the multipole interaction would produce superfluid nuclear needles. Magic nuclei are spherical despite the strong multipole interaction, because the large gaps in the nuclear mean field at the Fermi surface block the correlations.

Lets consider a simple model in which the valence space only contains two Slater determinants which have diagonal energies that differ by Δ and an off-diagonal matrix element δ. The eigenvalues and eigenvectors of this problem are obtained diagonalizing the matrix:

$$\begin{pmatrix} 0 & \delta \\ \delta & \Delta \end{pmatrix} \tag{51}$$

In the limit $\delta << \Delta$ we can use perturbation theory and no special coherence is found. On the contrary in the degenerate case, $\Delta \rightarrow 0$, the eigenvalues of the problem are $\pm\delta$ and the eigenstates are the 50% mixing of the unperturbed ones with different signs. They are the germ of the maximally correlated (or anticorrelated) states.

We can generalize this example by considering a degenerate case with N Slater determinants with equal (and attractive) diagonal matrix elements (– Δ) and off-diagonal ones of the same magnitude. The problem now is that of diagonalizing the matrix:

$$-\Delta \begin{pmatrix} 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & \dots \\ . & . & . & \dots \\ . & . & . & \dots \\ . & . & . & \dots \end{pmatrix} \tag{52}$$

which has range 1 and whose eigenvalues are all zero except one which has the value -NΔ. This is the coherent state. Its corresponding eigenvector is a mixing of the N unperturbed states with amplitudes $\frac{1}{\sqrt{N}}$

X. NUCLEAR SUPERFLUIDITY: PAIRING COLLECTIVITY

The pairing hamiltonian for one shell expressed in the m-scheme basis of two particles has a very similar matrix representation;

$$-G\begin{pmatrix} 1 & -1 & 1 & \dots \\ -1 & 1 & -1 & \dots \\ 1 & -1 & 1 & \dots \\ . & . & . & \dots \\ . & . & . & \dots \\ . & . & . & \dots \end{pmatrix} \tag{53}$$

and its coherent solution is just the state of the two particles coupled to zero which gains an energy -GΩ, (Ω= j + 1/2 is the degeneracy of the shell). It can be written as:

$$Z_j^\dagger|0\rangle = \frac{1}{\sqrt{\Omega}}\sum_{m>0}(-1)^{j+m}a_{jm}^\dagger a_{j-m}^\dagger \tag{54}$$

Using the commutation relations:

$$\left[Z_j, Z_j^\dagger\right] = 1 - \frac{\hat{n}}{\Omega}; \text{ and } \left[H, Z_j^\dagger\right] = -G(\Omega - \hat{n} + 2)Z_j^\dagger \tag{55}$$

it is possible to construct the eigenstates of H for n particles consisting of n/2 pairs coupled to J=0. These states are labeled as seniority zero states. The quantum number v (seniority) counts the number of particles not coupled to zero.

$$|n, v=0\rangle = (Z_j^\dagger)^{\frac{n}{2}}|0\rangle \text{ and } E(n, v=0) = -\frac{G}{4}n(2\Omega - n + 2) \tag{56}$$

We can construct also eigenstates with higher seniority using the operators $B_J^\dagger$ which create a pair of particles coupled to J≠0. These operators satisfy the relation:

$$\left[H, B_J^\dagger\right]|0\rangle = 0 \tag{57}$$

States which contain m $B_J^\dagger$ operators have seniority $v = 2m$. Their eigenenergies are,

$$E(n, v) - E(n, v=0) = \frac{G}{4}v(2\Omega - v + 2) \tag{58}$$

Notice that the gap is independent of the number of particles. The generalization to odd number of particles is trivial.

For n protons and neutrons in the same shell of degeneracy Ω coupled to total isospin T and reduced isospin t, the eigenvalues of the J=0 (L=0) T=1 pairing hamiltonian can be written as:

$$E(\Omega, n, v, t, T) = -G((n-v)(4\Omega + 6 - n - v)/8 + t(t+1)/2 - T(T+1)/2) \tag{59}$$

The case of two particles in several shells is also tractable and has great heuristic value. The problem in matrix form reads:

$$\begin{pmatrix} 2\epsilon_1 - G\Omega_1 & -G\sqrt{\Omega_1\Omega_2} & -G\sqrt{\Omega_1\Omega_3} & \dots \\ -G\sqrt{\Omega_2\Omega_1} & 2\epsilon_2 - G\Omega_2 & -G\sqrt{\Omega_2\Omega_3} & \dots \\ -G\sqrt{\Omega_3\Omega_1} & -G\sqrt{\Omega_3\Omega_2} & 2\epsilon_3 - G\Omega_3 & \dots \\ . & . & . & \dots \\ . & . & . & \dots \\ . & . & . & \dots \end{pmatrix} \tag{60}$$

There is a limit in which maximum coherence is achieved; when the orbits have the same Ω and they are degenerate. Then the coherent pair is evenly distributed among the shells and its energy is E=-G $\sum_i \Omega$. All the other solutions remain at their unperturbed energies.
A textbook case of nuclear superfluidity is provided by the Tin isotopes fro N=52 to N=80. The five orbits comprised between the magic closures 50 and 82 are closely packed and one should expect pairing dominance in several shells. The pairing gap is measured by the excitation energy of the first 2^+ state and should be independent of the neutron number. Indeed that is what the experiments tell us and what the SM-CI calculations reproduce nicely as can be seen in Figure 5.

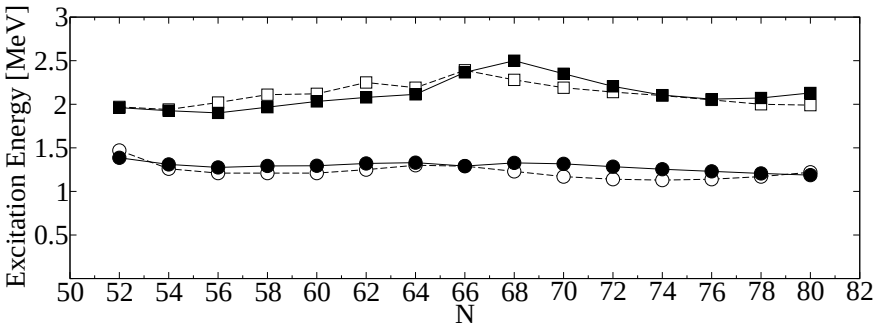


FIG. 5. Low energy excites states of the Tin isotopes; experiment *vs* SM calculations in the r_4h space with the gcn50:82 interaction; 2^+ circles, 4^+ squares, th. (filled) exp. (empty)

The problem can be turned into a dispersion relation as well. Let us write the most general solution as:

$$|\alpha\rangle = \sum_j X_j^\alpha Z_j^\dagger |0\rangle \tag{61}$$

Plugging it in the Schrödinger equation; $H|\alpha\rangle = E_\alpha|\alpha\rangle$ we get,

$$(2\epsilon_k - E_\alpha)X_k^\alpha = G\sum_j \sqrt{\Omega_j\Omega_k}X_j^\alpha \tag{62}$$

Multiplying by $\sqrt{\Omega_k}$ both sides and summing over k we obtain the dispersion relation:

$$\frac{1}{G} = \sum_k \frac{\Omega_k}{2\epsilon_k - E_\alpha} \tag{63}$$

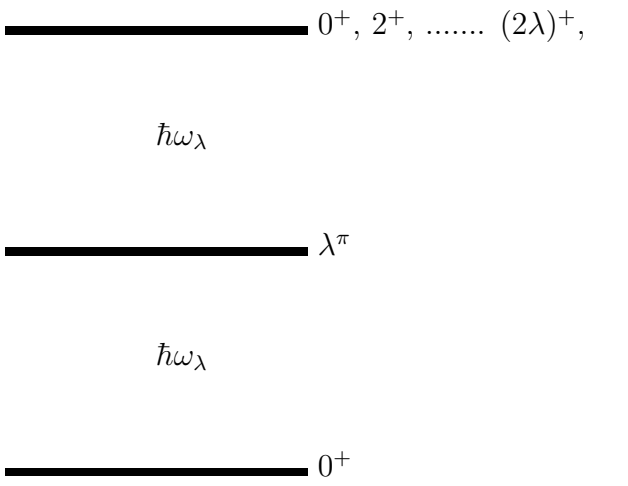
The dispersion relation can be solved graphically or iteratively. As we have seen before, we expect one coherent solution (the collective pair) to gain a lot of energy and the rest of the solutions be very close to the unperturbed ones. If we assume that the single particle energies are degenerate and take $\epsilon_k =< \epsilon >$ we obtain,

$$E_\alpha = 2 < \epsilon > -G\sum_k \Omega_k \tag{64}$$

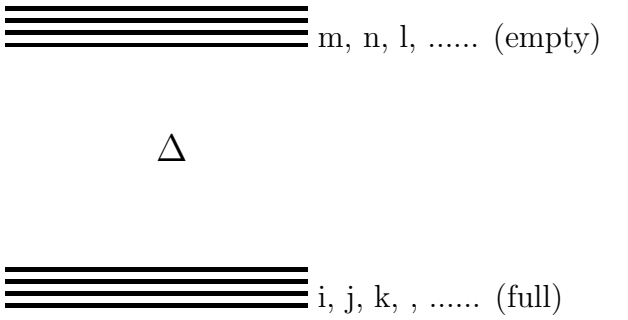
In this limit the energy gain is equivalent to the one in a single shell of degeneracy $\sum_k \Omega_k$
For the case of many particles in non degenerate orbits the problem is usually solved in the BCS or Hartree-Fock Bogolyuvov approximations. Other approaches, which do not break the particle number conservation, are either the Interacting Shell Model or are based on it, these include the Interacting Boson Model and its variants and different group theoretical approximations.

XI. VIBRATIONAL SPECTRA: QUADRUPOLE AND OCTUPOLE COLLECTIVITY.

In the semiclassical description, vibrational spectra are described as the quantized harmonic modes of vibration of the surface of a liquid drop. The restoring force coming from the competition of the surface tension and the Coulomb repulsion. This is hardly germane to reality and to the microscopic description that we will develop in a simplified way. Let's just remind which are the characteristic features of a nuclear vibrator; first, a harmonic spectrum such as in the drawing below and second, enhanced Eλ transitions between the states differing in one vibrational phonon.



Imagine that for a given even-even nucleus the orbits around the Fermi level are such as depicted in the graph below. Its ground state would have $J^\pi = 0^+$ and, in the IPM, the lowest excited states correspond to promoting one particle from the occupied orbits to the empty ones. They are many, quasi-degenerate, and should appear at excitation energies Δ.



Let's take now into account the multipole hamiltonian, that, for simplicity will be of separable form, and choose as valence space just the particle-hole states,

$$\langle nj|V|mi\rangle = \beta_\lambda Q^\lambda_{nj} Q^\lambda_{mi} \tag{65}$$

the wave function can be developed in the p-h basis as:

$$\Psi = \sum C_{mi}|mi\rangle \tag{66}$$

the Schödinger equation HΨ=EΨ can thus be written as:

$$C_{nj}(E - \epsilon_{nj}) = \sum_{mi} \beta_\lambda C_{mi} Q^\lambda_{nj} Q^\lambda_{mi} \tag{67}$$

then,

$$C_{nj} = \frac{\beta_\lambda Q^\lambda_{nj}}{E - \epsilon_{nj}} \sum_{mi} C_{mi} Q^\lambda_{mi} \tag{68}$$

and, trivially,

$$1 = \beta_\lambda \sum_{nj} \frac{(Q^\lambda_{nj})^2}{E - \epsilon_{nj}} \tag{69}$$

A graphical analysis of this equation (Figure 6) shows that all its solutions except one are very close to the unperturbed values ϵ_{nj}, the remaining one is the lowest and it is well separated from the others, very much as in the pairing case discussed before. Assuming

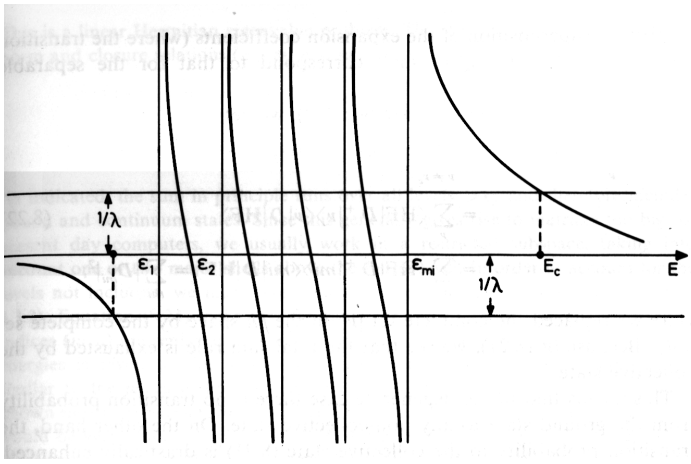


FIG. 6. Graphical analysis of the dispersion relation of equation 69

$\epsilon_{nj} \approx \overline{\epsilon_{nj}} = \Delta$, we obtain:

$$E = \Delta + \beta_\lambda \sum_{nj} (Q^\lambda_{nj})^2 \tag{70}$$

If the interaction is attractive $\beta_\lambda < 0$, the lowest state gains an energy which is proportional to β_λ, the strength of the multipole interaction, and to the coherent sum of the squared one body matrix elements of the one body multipole operators between the particle and hole orbits in the space. This mechanism of coherence explains the appearance of vibrational states in the nucleus and represents the basic microscopic description of the nuclear "phonons". Because the couplings β_λ are constant except for a global scaling, the onset of collectivity requires the presence of several quasi degenerate orbits above and below the Fermi level. In addition, these orbits must have large matrix elements with the multipole operator of interest.

The wave function of the coherent (collective) state (phonon, vibration) has the following form:

$$\Psi_c(J = \lambda) = \frac{\sum_{nj} Q^\lambda_{nj} |nj\rangle}{\sum_{nj} (Q^\lambda_{nj})^2} \tag{71}$$

The coherent state is coherent with the transition operator Q^λ because the probability of its Eλ decay to the 0^+ ground state is very much enhanced

$$B(E\lambda) \sim |\langle 0^+ | Q^\lambda | \Psi_c(J = \lambda)\rangle|^2 = \sum_{nj} (Q^\lambda_{nj})^2 \tag{72}$$

which should be much larger than the single particle limit (many WU). Clearly, a large value of the $B(E\lambda)$ does not imply necessarily the existence of permanent deformation in the ground state. Notice also that nothing prevents that:

$$|\beta_\lambda \sum_{nj} (Q^\lambda_{nj})^2| > \Delta \tag{73}$$

In this case the vibrational phonon is more bound than the ground state and the model is no longer valid. What happens is that a phase transition from the vibrational to the rotational regime takes place as the nucleus acquires permanent deformation of multipolarity λ. The separation between filled and empty orbits does not hold any more and both have to be treated at the same footing.

XII. DEFORMED NUCLEI; INTRINSIC *vs.* LABORATORY FRAME APPROACHES

The route to the description of permanently deformed nuclear rotors bifurcates now into laboratory frame and intrinsic descriptions. The latter include the deformed shell model (Nilsson) and the Deformed Hartree- Fock approximation, plus the Beyond Mean Field approaches such as angular momentum projection and configuration mixing with the generator coordinate method. The former, the Interacting Shell Model and the group theoretical treatments of the quadrupole-quadrupole interaction like Elliott's SU(3) and its variants [10–12].

A case where the two approaches could be confronted was ^{48}Cr (four protons and four neutrons on top of ^{40}Ca) where an ISM description in the full pf-shell was for the first time

TABLE II. Quadrupole properties of the yrast band of ^{48}Cr

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

possible more than one decade ago [13]. The mean field intrinsic description was a Cranked Hartree Fock Bogolyuvov description using the Gogny force. The results are presented in Figure 7. Both calculations reproduce the rotor like behavior at low and medium spin and the existence of a 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.

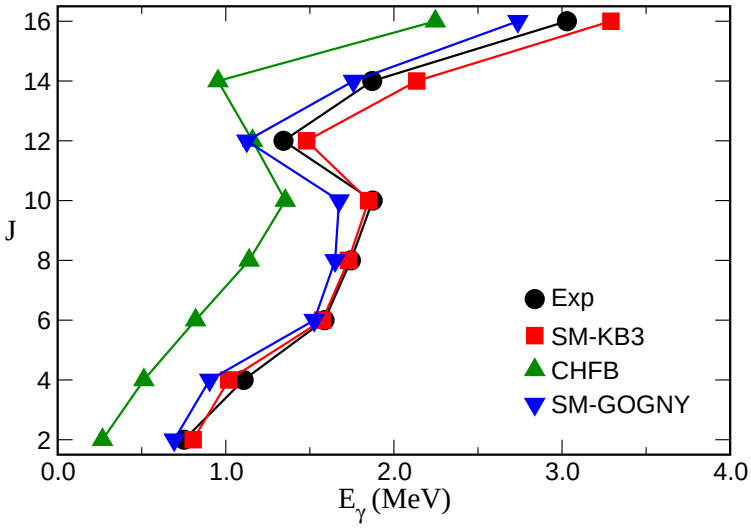


FIG. 7. The yrast band of ^{48}Cr; experimental data compared with the ISM and CHFB calculations.

The laboratory frame wave-functions are indeed collective as can be seen in Table II where we have listed the B(2)'s and spectroscopic quadrupole moments compared with the experiment. 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 a deformation parameter β=0.28 can be extracted which is in very good agreement with the CHFB result.

A. The Nilsson model

The Nilsson model is an approximation to the solution of the IPM plus a quadrupole-quadrupole interaction.

$$H = \sum_i h(\vec{r}_i) + \hbar\omega\kappa \sum_{i<j} Q_i \cdot Q_j$$

$$h(r) = -V_0 + t + \frac{1}{2}m\omega^2 r^2 - V_{so}\vec{l}\cdot\vec{s} - V_B l^2$$

Which amounts to linearizing the quadrupole quadrupole interaction, replacing one of the operators by the expectation value of the quadrupole moment (or by the deformation parameter). Thus, the resulting physical problem is that of the IPM subject to a quadrupole field, which, obviously breaks rotational symmetry.

$$H_{Nilsson} = \sum_i h(\vec{r}_i) - \frac{1}{3}\hbar\omega\delta Q_0(i)$$

The problem is equivalent to the diagonalization of the quadrupole operator in the basis of the IPM eigenstates. The resulting (Nilsson) levels are characterized by their magnetic projection on the symmetry axis m, also denoted K and the parity.

The formulae below make it possible to build the relevant matrices.

$$\langle pl|r^2|pl\rangle = p + 3/2 \quad : \quad \langle pl|r^2|pl+2\rangle = -[(p-l)(p+l+3)]^{1/2}$$

$$Q_0 = 2r^2 C_2 = 2r^2\sqrt{4\pi/(2l+1)}Y^{20} \quad : \quad \langle jm|C_2|jm\rangle = \frac{j(j+1)-3m^2}{2j(2j+2)}$$

$$\langle jm|C_2|j+2m\rangle = \frac{3}{2}\left\{\frac{[(j+2)^2-m^2][(j+1)^2-m^2]}{(2j+2)^2(2j+4)^2}\right\}^{1/2}$$

$$\langle jm|C_2|j+1m\rangle = -\frac{3m[(j+1)^2-m^2]^{1/2}}{j(2j+4)(2j+2)}$$

The intrinsic wave functions provided by the Nilsson model correspond to the Slater determinants built putting the neutrons and the protons in the lowest Nilsson levels (each one has degeneracy two, ±m). Therefore, for even even nuclei K=0, for odd nuclei K=m of the last half occupied orbit, and for odd-odd, there are different empirical rules, not always very reliable. The laboratory frame wave functions are obtained rotating the intrinsic frame with the Wigner matrices, i.e. correspond to the solutions of the rigid rotor problem. In the even-even case this leads trivially to the energy formula for a rotor:

$$E(J) = \sum_i \epsilon_i(Nilsson) + \frac{\hbar^2}{2\mathcal{I}}J(J+1)$$

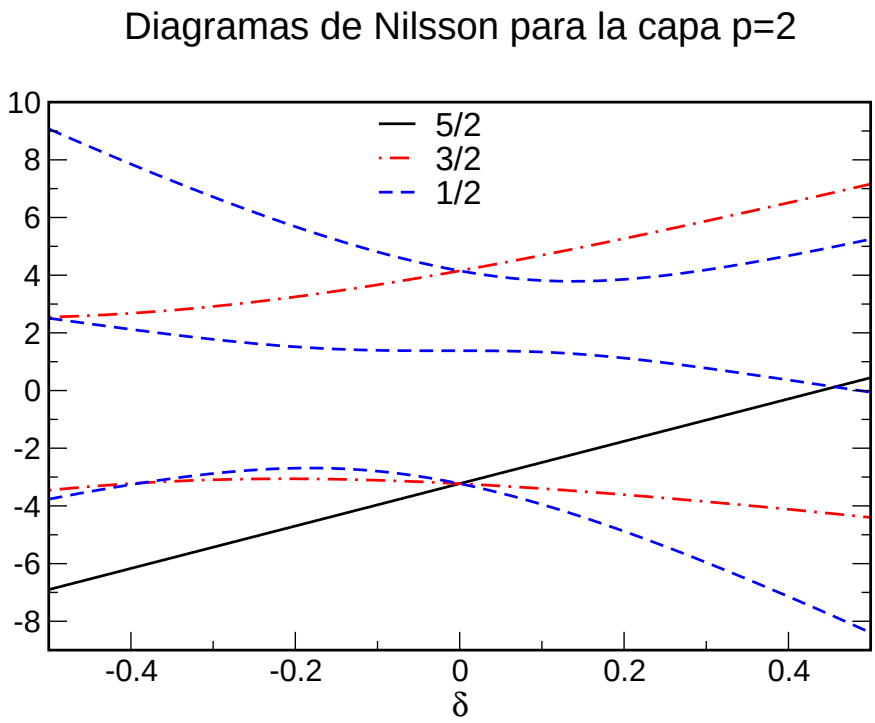


FIG. 8. Nilsson diagrams for the *sd*-shell; K=5/2 (black), K=3/2 (red), K=1/2 (blue)

B. The SU3 symmetry of the HO and Elliott's Model

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 harmonic oscillator (HO) shell; ii) the monopole hamiltonian makes the orbits of this shell degenerate 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 isotropic HO which in units m=1 ω=1 can be written as:

$$H_0 = \frac{1}{2}(p^2 + r^2) = \frac{1}{2}(\vec{p} + i\vec{r})(\vec{p} - i\vec{r}) + \frac{3}{2}\hbar = \hbar(\vec{A}^\dagger \vec{A} + \frac{3}{2}) \tag{74}$$

with

$$\vec{A}^\dagger = \frac{1}{\sqrt{2\hbar}}(\vec{p} + i\vec{r}) \quad \vec{A} = \frac{1}{\sqrt{2\hbar}}(\vec{p} - i\vec{r}) \tag{75}$$

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 built 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 in 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:

$$q_\mu^{(2)} = \frac{\sqrt{6}}{2\hbar}(\vec{r} \wedge \vec{r})_\mu^{(2)} + \frac{\sqrt{6}}{2\hbar}(\vec{p} \wedge \vec{p})_\mu^{(2)} \tag{76}$$

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 $n_1+n_2+n_3=N\mathbf{p}$ (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 N**p** 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 $3a+\lambda+2\mu=N\mathbf{p}$.

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

$$\vec{L} = \sum_{i=1}^{N} \vec{l}(i) \qquad Q_\alpha^{(2)} = \sum_{i=1}^{N} q_\alpha^{(2)}(i) \tag{77}$$

as:

$$C_{SU(3)} = \frac{3}{4}(\vec{L} \cdot \vec{L}) + \frac{1}{4}(Q^{(2)} \cdot Q^{(2)}) \tag{78}$$

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:

$$C(\lambda, \mu) = \lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu) \tag{79}$$

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

$$H = H_0 + \chi(Q^{(2)} \cdot Q^{(2)}) \tag{80}$$

which can be rewritten as:

$$H = H_0 + 4\chi C_{SU(3)} - 3\chi(\vec{L} \cdot \vec{L}) \tag{81}$$

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:

$$E(\lambda, \mu, L) = N\hbar\omega(p + \frac{3}{2}) + 4\chi(\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)) - 3\chi L(L + 1) \tag{82}$$

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

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)⊃O(3)⊃U(1) which corresponds to labeling the states as $\Psi([\tilde{f}](\lambda\mu)LM)$. $[\tilde{f}]$ is the representation of U(Ω) 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. The other chain of subgroups, SU(3)⊃SU(2)⊃U(1), does not contain O(3) and therefore the total orbital angular momentum is not a good quantum number anymore. Instead we can label the wave functions as; $\Phi([\tilde{f}](\lambda\mu)q_0\Lambda K)$, where q_0 is the intrinsic quadrupole moment whose maximum value is $q_0 = 2\lambda + \mu + 3$. 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:

$$\Psi([\tilde{f}](\lambda\mu)LM) = \frac{2L+1}{a(\lambda\mu KL)} \int D^L_{MK}(\omega)\Phi_\omega([\tilde{f}](\lambda\mu)(q_0)_{max}\Lambda K)d\omega \tag{83}$$

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.

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 $b^2 \approx 60$ efm^2. For ^{24}Mg we have (8,4) and 23 $b^2 \approx 70$ 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:

$$Q_0(s) = \frac{(J+1)\,(2J+3)}{3K^2 - J(J+1)}\, Q_{spec}(J), \quad K \neq 1 \tag{84}$$

$$B(E2, J \;\rightarrow\; J-2) = \frac{5}{16\pi}\, e^2 |\langle JK20|J-2, K\rangle|^2\, Q_0(t)^2 \quad K \neq 1/2,\, 1; \tag{85}$$

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) efm^2 and B(E2)($2^+\rightarrow 0^+$)=66(3) e^2fm^4 for ^{20}Ne and $Q_{spec}(2^+)$=–17(1) efm^2 and B(E2)($2^+\rightarrow 0^+$)=70(3) e^2fm^4 for ^{24}Mg.

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, this space has been denoted by r_p before. Its quadrupole properties are the SU(3) ones of 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 Δj=2, Δl=2; Δj=4, Δl=4; etc, orbits obtained from it. Its quadrupole properties are described in ref. [17]. 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. 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.

XIII. NUCLEAR DEFORMATION IN THE LABORATORY FRAME: CI-SM APPROACHES

Large Scale Shell Model calculations (LSSM), when doable, are the spectroscopic tool of choice in theoretical nuclear structure. When they are interpreted adequately they may provide us with the link between the experimental data and the "ab initio" approaches. Indeed, the monopole anomaly of the realistic NN interactions may turn out to be the fingerprint of residual three body effects [15, 16]. A non-negligible fraction of the Segré chart is nowadays amenable to LSSM descriptions. As explained in detail in [17] the choice of a valence space which can encompass the physics dictated by the effective interaction is the crucial one in SM work. Magic numbers provide the natural borders of the SM valence spaces, because they are supposed to correspond to large gaps in the spherical mean field. Nevertheless, sometimes, if the gaps are weakened this may not hold anymore.

Classical valence spaces associated to the harmonic oscillator (HO) closures are the *p*-shell and the *sd*-shell. Next comes the *pf*-shell, but it is well known that 40 is not a good magic number in general. In the *pf*-shell there is a transit from the HO closures to the spin-orbit ones (SO). The SO magic numbers are 6, 14, 28, 50, 82, and 126. They suggest valence spaces called extruder-intruder (EI). The exception is the lower *pf*-shell (N,Z $\leq$34) in which the optimal valence space is still the **p**=3 HO major shell. The EI valence spaces comprise all the orbits in major HO shell of principal quantum number **p** except the one with maximum angular momentum j=**p** +1/2, denoted by **rp**, plus the orbit j= **p+1**+1/2, brought down in energy from the next HO shell by the spin-orbit interaction. We use sometimes the notation **rpl**, (**l=p+1**) for these valence spaces; for instance **r3g** has a core N=Z=28 and spans till N=Z=50. EI spaces must be extended when quadrupole correlations are very strong. The resulting EEI include the quadrupole partner (or partners) of the intruder orbit, *e. g.* the EEI space corresponding to the r3g EI should incorporate (at least) the $1d_{5/2}$ orbit.

The *pf*-shell provides a valence space which can cope (and with flying colors) with the physics of several N=Z nuclei. From the point of view of the quadrupole coupling schemes which will be deal with in the next section, ^{48}Cr and ^{52}Fe are good quasi-SU3 deformed nuclei. ^{56}Ni is doubly magic albeit the closed shell amounts just to 60%-70% depending on the calculations. ^{60}Zn is transitional and ^{64}Ge looks very much like a pseudo-SU3 mildly deformed nucleus. Beyond, we need to change the valence space.

The next valence space is of EI type, **r3g**, comprising the orbits $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$, and $0g_{9/2}$. ^{68}Se is a natural inhabitant of this space. However, the region of applicability of this valence space at or close to N= Z will not extend very far. Already at ^{72}Kr, oblate prolate coexistence sets in, demanding that the quadrupole partner of the $0g_{9/2}$ orbit, $1d_{5/2}$, be included as well [21]. This leads to the EEI *r*3*gd* space. The next (and last) doubly magic N=Z nucleus ^{100}Sn will be the core of another EI valence space, r4h, which spans between the magic numbers 50 and 82.

XIV. THE QUADRUPOLE INTERACTION: INTRINSIC STATES AND COHERENCE

In order to gauge the quadrupole coherence of a given nucleus, it is customary to compare its quadrupole properties with perfect Bohr Mottelson rotors, *i. e.* to verify that the E2

transition rates and the spectroscopic quadrupole moments of the states of the yrast band can be derived from a single intrinsic quadrupole moment using the formulas:

$$Q_{spec}(J) =< JJ|3z^2 - r^2|JJ > \tag{86}$$

$$Q_{0s} = \frac{(J+1)\,(2J+3)}{3K^2 - J(J+1)}\,Q_{spec}(J), \quad K \neq 1 \tag{87}$$

$$B(E2, J \;\rightarrow\; J-2) = \frac{5}{16\pi}\,e^2|\langle JK20|J-2,K\rangle|^2\,Q_{0t}^2 \quad K \neq 1/2,\,1 \tag{88}$$

If $Q_{0s} \approx Q_{0t}$ and constant, we can speak of good rotors. The excitation energies of the yrast band should be close to J(J+1) as well. However, in light and medium mass nuclei, pairing might distort the lower part of the spectrum, giving extra binding to the 0^+ ground states. It is therefore advisable to verify the J(J+1) law excluding the ground state. Another caveat here has to do with the (bad) habit of extracting from the B(E2) values deformation parameters β in cases in which the existence of an intrinsic deformed state is not guaranteed.

Quadrupole coherence may be associated with a single shell (Eq.(4)), with a full **rp**-shell (pseudo SU3) and in this case the intrinsic single particle states are obtained diagonalizing the quadrupole operator using using Eqs.(4, 5, 6)) or with a full HO major shell, thus the Nilsson-like orbits of Elliott's SU3 [18] obtain. If done in the $\Delta j = 2$ HO sequences (quasi SU3), one can diagonalize using Eqs.(4, 6) or the corresponding expressions in LS coupling as adopted in ref. [19]. We shall work with the latter choice. We use adimensional r^2, and $Q_0 = 2r^2C_2$. An quadrupole effective charges equal 0.5 and 1.5 for neuters and protons are used throughout this notes.

$$\begin{aligned}
\langle pl|r^2|pl\rangle &= p + 3/2 \\
\langle pl|r^2|pl+2\rangle &= -[(p-l)(p+l+3)]^{1/2} \\
\langle jm|C_2|jm\rangle &= \frac{j(j+1) - 3m^2}{2j(2j+2)}
\end{aligned} \tag{89}$$

$$\langle jm|C_2|j+1m\rangle = -\frac{3m[(j+1)^2 - m^2]^{1/2}}{j(2j+4)(2j+2)} \tag{90}$$

$$\langle jm|C_2|j+2m\rangle = \frac{3}{2}\left\{\frac{[(j+2)^2 - m^2][(j+1)^2 - m^2]}{(2j+2)^2(2j+4)^2}\right\}^{1/2} \tag{91}$$

To recover dimensions; $r^2 \rightarrow r^2b^2$.

A. 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:

$$\frac{Q_0}{b^2} = \sum_m 2r^2\langle jm|C_2|jm\rangle = \sum_m (p+3/2)\frac{j(j+1) - 3m^2}{j(j+1)} \tag{92}$$

TABLE III. Intrinsic quadrupole moments for n particles in the $0g_{9/2}$ orbit and N=Z (in units of b^2)

n	2	4	6	8	10	12	14	16	18
prol	5.33	10.66	14.66	18.66	20	21.33	18.66	16	8
-ob	8	16	18.66	21.33	20	18.66	14.66	10.66	5.33

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. In Table III, we list the Q_0 values for the $0g_{9/2}$ orbit and N=Z. 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.

B. SU(3) and pseudo-SU(3)

For a full HO shell, $Q_0 = 2n_z - n_x - n_z$, with $n_x + n_y + n_z = \mathbf{p}$. For $\mathbf{p}$=2, the intrinsic states are $[n_z n_x n_y]$=[200],[110],[101],[020],[011],[002]. The quadrupole moments of these states for the $\mathbf{p}$=2 and $\mathbf{p}$=4 shells are plotted in Fig. 9 (for $\mathbf{p}$=4 the values in the y-axis are -8, -5. -2, +1, +4). Now, orderly fillings in the figure produce eigenstates of $qq - \lambda L(L+1)$ and *a fortiori* rotational bands

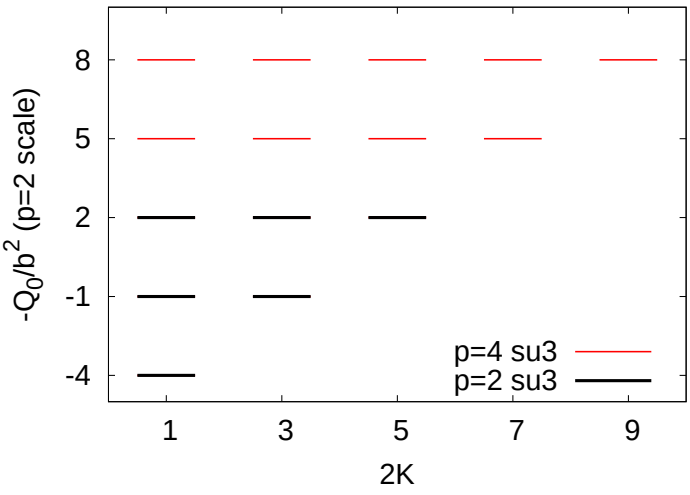


FIG. 9. Intrinsic states of SU3 for the p=2 and p=4 HO shells, the latter are scaled to the p=2 values

The values in a pseudo-SU(3) space [20] in shell $\mathbf{p}$ are approximately the ones of SU(3) in shell **p-1** multiplied by factors in the range (p+3/2)/(p+1/2) and $\sqrt{(p+4)/p+2)}$. In Figure 10 we have plotted the intrinsic states of pseudo-SU3 for the $r3$ valence space compared with those of SU3 in the $\mathbf{p}$=2 HO shell. Notice that the lowest prolate states have quadrupole moments that are about 20% larger than the SU3 ones for $\mathbf{p}$=2.

In Table IV we list the intrinsic quadrupole moments for n holes in r3 for later use. Only the oblate solutions are explicitly included. To get the prolate ones, take for n holes the oblate value for 24-n and change sign.

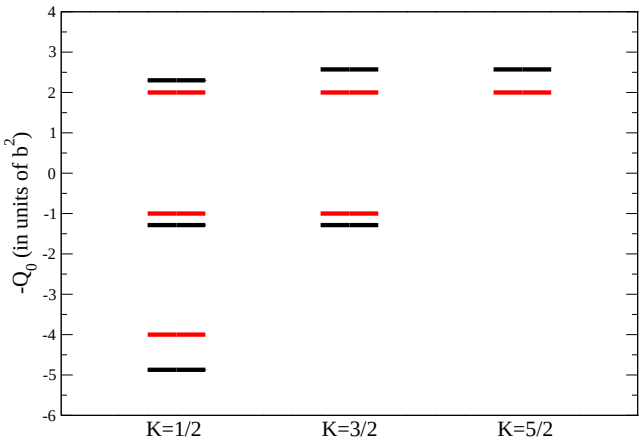


FIG. 10. Intrinsic states of pseudo-SU3 for the $r3$ valence space (black) compared with those of SU3 in the p=2 HO shell (red).

TABLE IV. Intrinsic quadrupole moments for n holes in r3 in the pseudo-SU3 limit (in units of b^2)

n	0	2	4	6	8	10	12
-psu3(o)	0.0	9.742	19.484	22.056	24.648	27.200	29.772
n	24	22	20	18	16	14	
-psu3(o)	0.0	5.142	10.284	15.426	20.568	25.170	

C. Quasi-SU3

In the case of a Δj=2 HO sequence, the resulting scheme is very much like that of SU(3) except that some degeneracies are not present and the quadrupole collectivity is a bit smaller as shown in Fig. 11.

In Table V we have listed the intrinsic quadrupole moments for n particles in the quasi-SU(3) sector of the **p**=4 HO shell. Only the prolate cases are considered. In reality in all the SU3-like cases the total intrinsic quadrupole moment obtained from these eigenvalues, has to be increased by 3 b^2 as explained in ref. [22].

TABLE V. Intrinsic quadrupole moments for n particles in the quasi-SU(3) sector of the **p**=4 HO shell

n	2	4	6	8	10	12	14	16	18
qsu3(p)	15	30	39	48	51	54	57	60	57

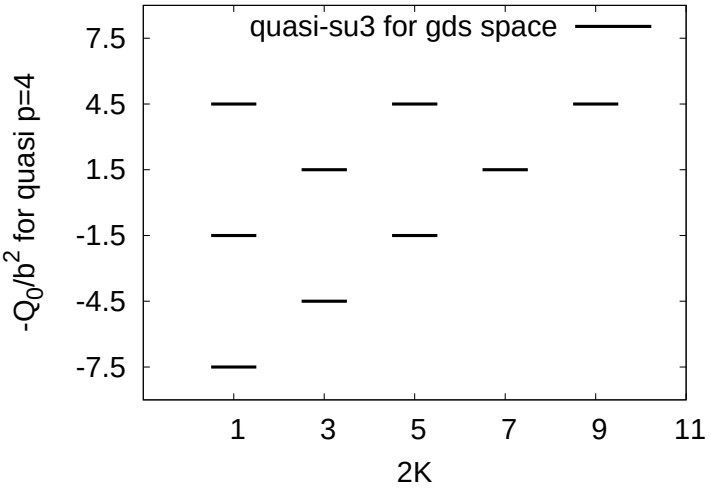
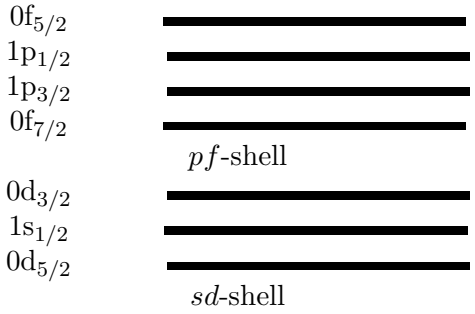


FIG. 11. Intrinsic states of quasi-SU3 for the p=4 HO shell

D. Coexistence: Spherical, Deformed and Superdeformed states in ^{40}Ca

Let's describe the structure of ^{40}Ca with a SM-CI calculation in the valence space of two major shells and interpret the results in the framework of SU(3) and its variants. The orbits of the valence space are sketched below



The relevant configurations are: $[sd]^{24}$ 0p-0h, spherical, $[sd]^{20}$ $[pf]^4$ 4p-4h, deformed, and $[sd]^{16}$ $[pf]^8$ 8p-8h, superdeformed.

The results presented in Fig. 12 show clearly the importance of the correlations. In the 8p-8h configuration the correlations amount to 18.5 MeV. 5.5 MeV are due to pairing and the remaining 13 MeV are most likely of quadrupole origin. In the 4p-4h configuration, the pairing contribution is similar, but the quadrupole is smaller at about 4.5 MeV. The closed shell gains 5 MeV of pairing energy by mixing (30%) with the 2p-2h states, the ND bandhead 2 MeV, and the SD bandhead essentially nothing.

Concerning the character of these solutions, we can see that for the 4p-4h intrinsic state of ^{40}Ca, the two neutrons and the 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 to the intrinsic quadrupole moment of Q_0=25 b^2. In the pseudo-sd shell, p=1 we are left with eight particles, that contribute with Q_0=7 b^2. In the 8p-8h the values are Q_0=35 b^2 and Q_0=11 b^2 Using the proper values of the oscillator length it obtains:

- ^{40}Ca 4p-4h band Q_0=125 e fm^2

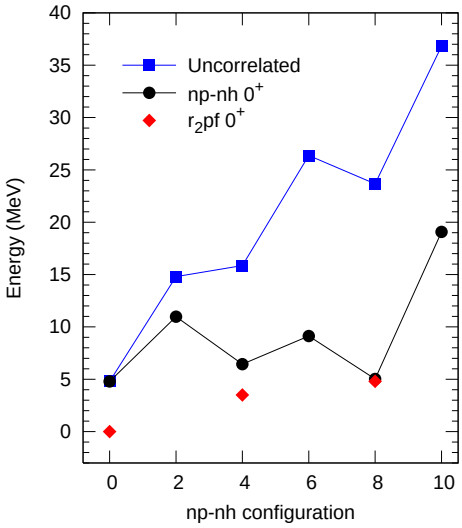


FIG. 12. Energies of the np-nh configurations; uncorrelated energies (blue); full mixing at fixed np-nh (black); full mixing (red)

- ^{40}Ca 8p-8h band Q_0=180 e fm^2

In very good accord with the data (Q_0=120 e fm^2 and Q_0=180 e fm^2). Assuming full SU3 symmetry in both shells we should get Q_0=148 e fm^2 and Q_0=226 e fm^2 respectively. The SM results almost saturate the quasi-SU3 bounds. The SU3 values are a 25% larger. Finally we compare the SM-CI results with experiment in Figure 13. The agreement is extremely satisfactory.

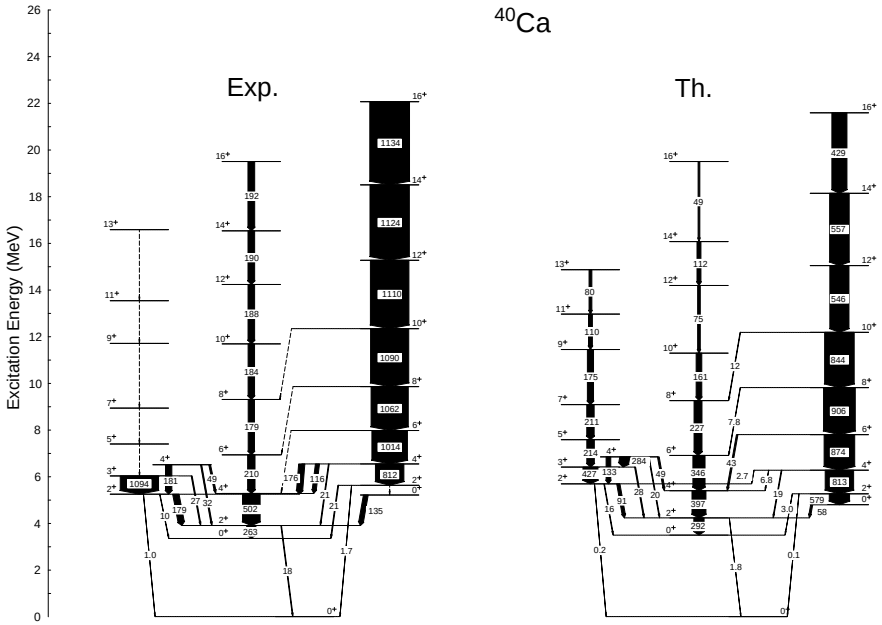


FIG. 13. Partial level scheme of ^{40}Ca; experiment vs large scale shell model results [8]

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For the less standard aspects of the presentation I follow the work of the Strasbourg Madrid Shell Model collaboration, notably the review of reference [17] (with special thanks to E. Caurier, G. Martínez-Pinedo, F. Nowacki, and A. P. Zuker).

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