The Shell Model: An Unified Description of the Structure of the Nucleus (III)

ALFREDO POVES

Departamento de Física Teórica and IFT, UAM-CSIC

Universidad Autónoma de Madrid (Spain)

”Frontiers in Nuclear and Hadronic Physics”

Galileo Galilei Institute

Florence, February-Mars, 2016

Understanding the Effective Nuclear 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 rule

Any effective interaction can be split in two parts:

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

$\mathcal{H}_m$ 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. this can be generalized the case of three body forces

A theorem

- Let's Ψ be an Slater determinant corresponding to filled HF spherical orbits
- Then, for a general general hamiltonian $\mathcal{H}$

$$< \Psi|\mathcal{H}|\Psi >$$

- Depends only on the occupation numbers of the IPM orbits. In the case of two body interaction it includes linear and quadratic terms.

Two representations of the Hamiltonian

$\mathcal{H}$ can be written in two representations, particle-particle and particle-hole (r s t u label orbits; Γ and γ are shorthands for (J,T))

$$\mathcal{H} = \sum_{r\leq s, t\leq u, \Gamma} W^{\Gamma}_{rstu} Z^{+}_{rs\Gamma} \cdot Z_{tu\Gamma},$$

$$\mathcal{H} = \sum_{rstu\Gamma} [2\gamma+1]^{1/2} \frac{(1+\delta_{rs})^{1/2}(1+\delta_{tu})^{1/2}}{4} \omega^{\gamma}_{rtsu} (S^{\gamma}_{rt} S^{\gamma}_{su})^{0},$$

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.

$$Z^{+}_{rs\Gamma} = [a^{\dagger}_{r} a^{\dagger}_{s}]^{\Gamma} \text{ and } S^{\gamma}_{rs} = [a^{\dagger}_{r} a_{s}]^{\gamma}$$

Two representations of the Hamiltonian

The W and ω matrix elements are related by a Racah transformation (there is an implicit product of the ordinary and isospin space coefficients here)

$$\omega_{rtsu}^{\gamma} = \sum_{\Gamma} (-)^{s+t-\gamma-\Gamma} \left\{ \begin{array}{ccc} r & s & \Gamma \\ u & t & \gamma \end{array} \right\} W_{rstu}^{\Gamma} [2\Gamma + 1],$$

$$W_{rstu}^{\Gamma} = \sum_{\gamma} (-)^{s+t-\gamma-\Gamma} \left\{ \begin{array}{ccc} r & s & \Gamma \\ u & t & \gamma \end{array} \right\} \omega_{rtsu}^{\gamma} [2\gamma + 1].$$

The operators $S_{rr}^{\gamma=0}$ are just the number operators for orbits r and $S_{rr'}^{\gamma=0}$ the spherical HF particle hole vertices. The latter must have null coefficients if the monopole hamiltonian satisfies HF self-consistency. The former produce the Monopole Hamiltonian

The Monopole Hamiltonian

$$\mathcal{H}_m = \sum_{i,\rho=\nu,\pi} \epsilon_{i,\rho}\hat{n}_{i,\rho} + \sum_{ij,\rho\rho'} \left[\frac{1}{(1+\delta_{ij}\delta_{\rho\rho'})} V_{ij}^{\rho\rho'}\, \hat{n}_{i\rho}(\hat{n}_{j\rho'} - \delta_{ij}\delta_{\rho\rho'}) \right]$$

The centroïds $V_{ij}^{\rho\rho'}$ are angular averages of the two body matrix elements of the neutron-neutron, proton-proton and neutron-proton interactions.

$$V_{ij} = \frac{\sum_J W_{ijij}^J [2J+1]}{\sum_J [2J+1]}$$

The sums run over Pauli allowed values,.

The expectation value of the Hamiltonian with a single Slater Determinant (closed orbits)

It is easy to verify that the expectation value of the full Hamiltonian in a Slater determinant for closed shells, or equivalently, the energy in the Hartree-Fock approximation is:

$$\langle H \rangle = \sum_i \langle i|T|i\rangle + \sum_{ij} \langle ij|W|ij\rangle$$

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:

$$\langle H \rangle = \sum_\alpha (2j_\alpha + 1)\langle \alpha|T|\alpha\rangle + \sum_{\alpha\leq\beta}\sum_{J,T}(2J+1)(2T+1)\langle j_\alpha j_\beta (JT)|W|j_\alpha j_\beta (JT)\rangle$$

Which is just the expectation value of the Monopole Hamiltonian,

The Monopole Hamiltonian and Shell Evolution

The evolution of effective spherical single particle energies (ESPE's) with the number of particles in the valence space is dictated by $\mathcal{H}_m$. Schematically:

$$\epsilon_k(\{n_i, n_j, \ldots\}) = \epsilon_k(\{n_i^0, n_j^0, \ldots\}) + \sum_m V_{km} n_m + \sum_{i,j} \mathcal{V}_{kij} n_i n_j$$

This expression shows clearly that the underlying spherical mean field is "CONFIGURATION DEPENDENT"

It also shows 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

- 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) produces a $(\vec{\sigma}\cdot\vec{\sigma})$ $(\vec{\tau}\cdot\vec{\tau})$ term which is nothing 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 effective nucleon-nucleon interaction in the nucleus, 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 $(r^{\lambda}Y_{\lambda}\cdot r^{\lambda}Y_{\lambda})$

The Effective Interaction

The evolution of the spherical mean field in the valence spaces remains a key issue, because we know since long that something is missing in the monopole hamiltonian derived from the realistic NN interactions, be it through a G-matrix, V_{low-k} or other options.

The need for three body forces is now confirmed. Would they be reducible to simple monopole forms? Would they solve the monopole puzzle of the ISM calculations? The preliminary results seem to point in this direction

The multipole hamiltonian does not seem to demand major changes with respect to the one derived from the realistic nucleon-nucleon potentials and this is a real blessing because it suggest that the effect of the three body interactions in the many nucleon system may be well approximated by monopole terms

Heuristics of the Effective interaction

- We start with the effective interaction given by its single particle energies a two body matrix elements
- And extract the monopole hamiltonian $\mathcal{H}_m$
- Next the isovector and isoscalar pairing, $\mathcal{P}_{01}$, $\mathcal{P}_{10}$
- We change now to the particle-hole representation, dominated by the quadrupole-quadrupole interaction
- In the actual calculations we must use the full interaction, but, for the heuristic which follows we may use the schematic version
- $\mathcal{H}_m + \mathcal{P}_{01} + \mathcal{P}_{10} + \sum_\lambda \beta^\lambda\, Q^\lambda \cdot Q^\lambda$

Collectivity in Nuclei

- 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.
- If 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
- In the extreme limit in which the monopole hamiltonian is 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

Coherence; basic notions

- 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:

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

- 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

Coherence; basic notions

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

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

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

Nuclear superfluidity: pairing in one orbit

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

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

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

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

Nuclear superfluidity: pairing in one orbit

- Using the commutation relations:

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

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

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

Nuclear superfluidity: pairing in one orbit

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

$$\left[H, B_J^\dagger\right]|0\rangle = 0$$

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

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

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

Nuclear superfluidity: pairing in one orbit for protons and neutrons

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

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

Nuclear superfluidity: two particles in several orbits

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

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

- 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 them and its energy is E=-G $\sum_i \Omega$. All the other solutions remain at their unperturbed energies.

Nuclear superfluidity: two particles in several orbits

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

$$|\alpha\rangle = \sum_j X_j^\alpha Z_j^\dagger |0\rangle$$

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

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

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

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

Nuclear superfluidity: two particles in several orbits

- 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

$$E_\alpha = 2 < \epsilon > - G \sum_k \Omega_k$$

- In this limit the energy gain is equivalent to the one in a single orbit of degeneracy $\sum_k \Omega_k$

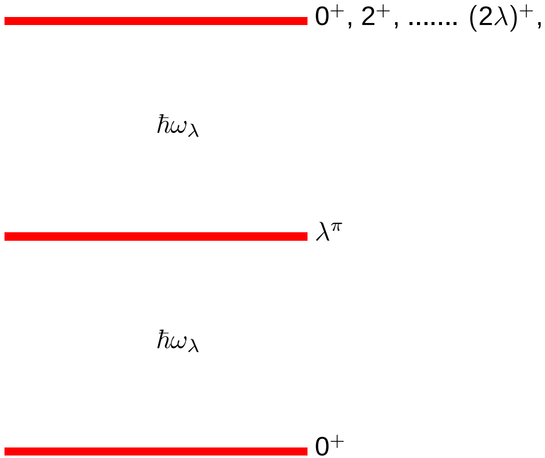
Nuclear superfluidity: the general case

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

Vibrational spectra

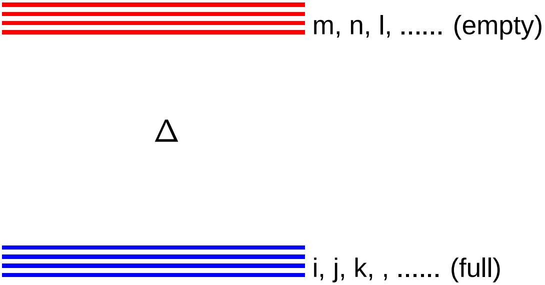
In the semiclassical description, vibrational spectra are described as the quantized harmonic modes of vibration of the surface of a liquid drop. The restoring force comes from the competition of the surface tension and the Coulomb repulsion. This is hardly germane to reality and to the microscopic description 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 figure and second, enhanced Eλ transitions between the states differing in one vibrational phonon.

Vibrational spectra



Vibrational spectra; The meaning of collectivity:

Imagine a situation such as depicted in the figure. The ground state has $J^{\pi} = 0^{+}$ and, in the IPM, the lowest excited states correspond to promoting one particle from the occupied orbits to the empty ones. There are many, quasi degenerate, and should appear at an excitation energy Δ.



The meaning of collectivity

Let's take now into account the multipole hamiltonian, that, for simplicity, will be of separable form, and restrict the valence space to the one particle one hole states

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

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

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

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

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

The meaning of collectivity

Then,

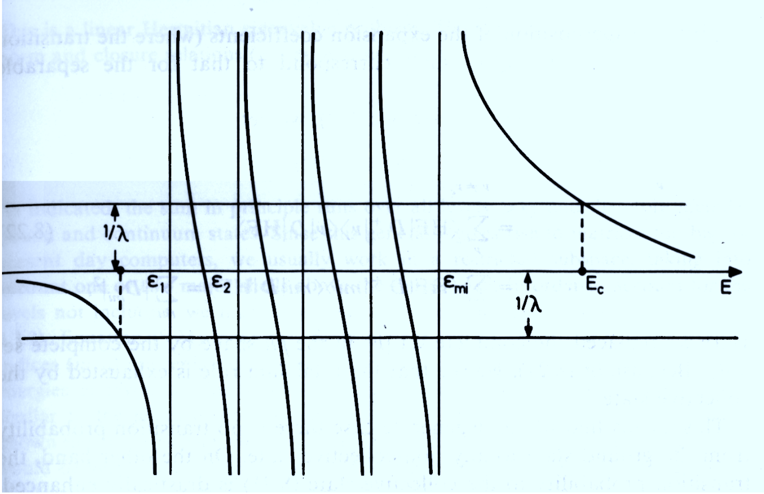
$$C_{nj} = \frac{\beta_\lambda Q_{nj}^\lambda}{E - \epsilon_{nj}} \sum_{mi} C_{mi} Q_{mi}^\lambda$$

and, trivially,

$$1 = \beta_\lambda \sum_{nj} \frac{(Q_{nj}^\lambda)^2}{E - \epsilon_{nj}}$$

A graphical analysis of this equation 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.

The meaning of collectivity



The meaning of collectivity

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

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

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".

The meaning of collectivity

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) (phonon) state has the following form:

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

The meaning of collectivity

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

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

Which should be much larger than the single particle limit (many WU). Notice that a large value of the $B(E\lambda)$ does not imply necessarily the existence of permanent deformation in the ground sate.

Shape transition; Deformed nuclei

Notice also that nothing prevents that:

$$|\beta_\lambda \sum_{nj} (Q_{nj}^{\lambda})^2| > \Delta$$

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 shells does not hold any more and both have to be treated at the same footing.

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 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.