The mean field approach to nuclear structure

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Abstract

This is the first version of the lecture notes of the mean field session of the course I taught at the Joliot Curie 2012 graduate school of nuclear physics. The theoretical aspects of the mean field description of the structure of the atomic nucleus are presented and discussed.

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I. INTRODUCTION

The atomic nucleus is a very complex microscopic system made of protons and neutrons [12][8][7]. The interaction among them is not a fundamental one, but the residual interaction among the constituents of the nucleon, namely quarks and gluons. This effective character is responsible for the complexity of the "nuclear force" and its exotic properties: it has a strong spin dependence, a strong tensor component, three body forces are relevant and it has a strongly repulsive core. In spite of all this complexity and the number of elements that make a typical nucleus (from a few nucleons to around three hundred) there is strong empirical evidence supporting the existence of a common potential that creates orbits occupied by the nucleon, very much the same as in the case of a standard atom where the electrons orbit around the central atomic nucleus. In the case of the nucleus there is no "natural center" and understanding the reason for such a common potential is a beautiful but extremely difficult exercise involving lots of quantum mechanics algebra. To make a long story short, is the Pauli principle that identical fermions have to obey, the responsible for protons and neutrons to stay away from each other in such a way that they only feel the long range mildly attractive part of the "nuclear potential". The most prominent experimental evidence in favor of a common potential is the existence of the so-called "magic numbers", a given set of proton or neutron numbers that imply extra stability at the level of binding energies. This phenomenon is also known in atomic physics in the form of the exceptional chemical stability of the noble gases. In terms of the simplistic view of the atom as made of a central nucleus with positive charge Z that creates an electrostatic potential, noble gases correspond to those electronic configurations that completely fill one of the orbitals created by the common potential. With this in mind, the extra stability of ^{208}Pb or ^{132}Sn, two double magic nuclei, shares the same explanation as the lack of chemical reactivity of Radon.

Pairing in another important piece of the nuclear puzzle: in a few words is the tendency protons and neutrons have to couple to "pairs" with angular momentum zero. This tendency explains, for instance some subtle differences in the binding energies of even-even nuclei (systems with an even number of protons and neutrons), odd-A ones (systems with either the number of protons or neutrons an odd number) or odd-odd systems and the result fundamental to explain the number of stable isotopes for a given chemical species. The existence of pairing interaction also explains in a very natural way the fact that the ground

state of all even-even nuclei is a 0^+ (i.e. angular momentum $J = 0$ and parity $\pi = +1$). The combination of the pairing ideas and the mean field potential is also fundamental to explain the spin and parity of odd-A systems in a natural way.

In the following I will describe how to handle the mean field and pairing concepts in a theoretical framework to describe the atomic nucleus. First, the concept of second quantization which is a useful tool to simplify the complicated quantum mechanisc algebra will be introduced. Next the focus will be in the description of the Hartree- Fock approximation which is the cornerstone of the mean field approximation. An example of application with a simplified model (Lipkin model) will be presented next. In the next section, the formalism used to combine the mean field and pairing concepts, namely the Hartree- Fock- Bogoliubov approximation will be discussed in detail. I will finish with some illustrative examples.

In the realm of the mean field, three different groups of effective interactions are popular: the Skyrme, Gogny and relativistic type of approaches. I will not dwell into the details that make each of the approaches different and refer the interested reader to the literature where there are abundant review articles [1][6][10].

II. SECOND QUANTIZATION FORMALISM

The second quantization formalism is a nice tool to simplify the description of a quantum mechanics system made up of many particles. The reader interested in a deeper understanding of the subject in a nuclear physics context can consult the textbooks of Refs [2][9] for more details. The mathematical description of a particle in the context of quantum mechanics is given in terms of a "vector state" belonging to a so-called Hilbert space (nothing but a vector space and a scalar product). Using Dirac's notation, vectors in the Hilbert space $\mathcal{H}$ are denoted by $|\alpha\rangle$ where α denotes a set of labels characterizing the state and depending on the physics to be described. To better understand this rather sophisticated mathematical language let us consider a quantum mechanic system made of a particle with a property that we will call "spin" taking only two possible values. The fact that only two values are enough to describe the system is given by its physical properties and obviously will change from system to system. In this case, the Hilbert space is the space of vectors in two dimensions and $|\alpha\rangle$is a linear combination of the two basic states corresponding to the two possible values (think in terms of spin up and spin down) represented by a vector with

two components

$$|\alpha\rangle = \alpha_1|\uparrow\rangle + \alpha_2|\downarrow\rangle = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}.$$

In the second example, we consider a particle in one dimension moving under the influence of a harmonic potential $V(x) = \frac{1}{2}m\omega^2 x^2$. In this case, the variable characterizing the particle is its position (and momentum) and therefore is a continuous variable. The states $|\alpha\rangle$ are linear combinations of states with a definite position $|x\rangle$

$$|\alpha\rangle = \int dx f_\alpha(x)|x\rangle$$

with functions $f_\alpha(x)$ having the property that $\int dx|f_\alpha(x)|^2 = 1$ (square integrable functions in mathematical jargon). The stationary states for this physical case are obtained by solving the Schrodinger equation leading to a set of infinite states $|n\rangle$characterized by an integer $n = 0, 1, \ldots$ The corresponding "wave functions" $f_n(x)$ are the well known wave functions of the harmonic oscillator in one dimension

$$\phi_n(x) = \mathcal{N}_n H_n(x/b)\exp(-\frac{1}{2}\frac{x^2}{b^2})$$

Those wave functions depend upon a length scale parameter b given in terms of the mass m and frequency ω of the oscillator. The generalization to three dimensions can be made in terms of three oscillators along each of the spatial directions leading to states characterized by the three quantum numbers n_x, n_y and n_z, that is one dimensional quantum numbers for each of the directions and a wave function

$$\phi_{n_x n_y n_z}(\vec{r}) = \phi_{n_x}(x)\phi_{n_y}(y)\phi_{n_z}(z)$$

Another possibility is to use spherical coordinates r, θ, ϕ instead of the cartesian ones x, y and z. In this case the quantum numbers are n, the radial quantum number, l the orbital angular momentum and m the projection of the angular momentum along the z axis

$$\Psi_{nlm}(\vec{r}) = R_{nl}(r)Y_{lm}(\theta, \phi)$$

Obviously, both sets of solutions of the Schroedinger equation are related by means of a unitary transformation and they represent different components of the same vector state expressed in different basis.

The above considerations can be extended to the case of many particle systems by considering wave functions of the A coordinates (and eventually spin and isospin) $\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_A)$.

When the A particles are indistinguishable (that is they have the same properties like mass, charge, spin, etc, like two protons) the symmetrization postulate of quantum mechanics has to be considered. In order to make the physical description of a system of A indistinguishable particles independent of the labeling of the particles it is necessary to impose that the A particle is either completely symmetric or skew-symmetric under the exchange of any two particles in the system. The postulate is complemented by a rule (some how justified in the context of quantum field theory) stating that particles with integer spin (or zero) must have symmetric wave functions whereas those particles with half integer spin (like the spin 1/2 protons and neutrons that constitute the atomic nucleus) must have completely skew-symmetric wave functions.

In the second quantization formalism a creation operator a_α^+ and the wave function of the vacuum $|\rangle$ are introduced in such a way that a vector state of a particle is given by the action of the creation operator in the vacuum

$$|\alpha\rangle = a_\alpha^+|-\rangle$$

that is, the operator a_α^+ creates a particle with quantum numbers α. A possible wave function of a system of two particles is given by the action of two creation operators in the vacuum

$$|\alpha_1\alpha_2\rangle = a_{\alpha_1}^+ a_{\alpha_2}^+|-\rangle.$$

This kind of wave function is denoted as "independent particle" wave functions as the wave functions of the two particles are independent of each other. This is not the most general type of two particle wave functions, that also includes fully correlated states like the general function $\Psi(\vec{r}_1, \vec{r}_2)$. However, any general function (satisfying the requirements of quantum mechanics) of the two coordinates can be expanded as a linear combination of "independent particle" wave functions

$$\Psi(\vec{r}_1, \vec{r}_2) = \sum_{\alpha_1\alpha_2} C_{\alpha_1\alpha_2}\phi_{\alpha_1}(\vec{r}_1)\phi_{\alpha_2}(\vec{r}_2)$$

indicating the relevant role played by those "independent particle" states. The procedure is easily extended to deal with the wave function of an A particle system. The "independent particle" type of wave functions is given in this case by the general product of A creation operators acting on the vacuum

$$|\alpha_1, \ldots, \alpha_N\rangle = \prod_{i=1}^{A} a^+_{\alpha_i}|-\rangle.$$

Along with the creation operators we have to consider they hermitian conjugate denoted a_α. This operators annihilate the vacuum

$$a_\alpha|-\rangle = 0$$

and, as discussed bellow, they also satisfy

$$a_\alpha a^+_\alpha|-\rangle = |-\rangle$$

that is easily interpreted by assigning to the operators a_α the role of annihilation operators of a particle in the quantum state α. Up to now nothing has been said about the symmetrization postulate of quantum mechanics. It turns out that it can be easily dealt with in the second quantization formalism by requiring that the creation and annihilation operators satisfy canonical commutation (anticommutation) relations for bosons (fermions). In the fermionic case (the one we are interested in) we have

$$\{a^+_\alpha, a^+_\beta\} = \{a_\alpha, a_\beta\} = 0 \,\text{and}\, \{a^+_\alpha, a_\beta\} = \delta_{\alpha\beta}$$

Operators depending on the properties of each particle, like the kinetic energy or the position operators are denoted as "one body operators" and are given by the sum of the corresponding operator acting on the appropriate Hilbert space

$$\hat{T} = \sum_{i=1}^{N} \hat{t}_i.$$

It turns out that those operators can be written in the second quantization formalism as

$$\hat{T} = \sum_{i=1}^{N} \hat{t}_i = \sum_{kl} t_{kl} a^+_k a_l$$

where t_{kl} are the operator's matrix elements between the states created by a^+_k and a^+_l

$$t_{kl} = \langle \phi_k|\hat{t}|\phi_l\rangle = \int d^3\vec{r}\, \phi^*_k(\vec{r})\hat{t}\phi_l(\vec{r}).$$

For instance, in the case of the momentum operator

$$\vec{P}_{kl} = i\hbar \int d^3\vec{r}\, \phi^*_k(\vec{r})\vec{\nabla}\phi_l(\vec{r}).$$

On the other hand, operators that depend on two particles, like the interaction potential, are denoted as two body operators

$$\hat{V} = \sum_{i<j} \hat{v}(i,j)$$

and given in the second quantization formalism by the expression

$$V = \sum_{i<j} v(i,j) = \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} \tilde{v}_{k_1 k_2 k_3 k_4} a^+_{k_1} a^+_{k_2} a_{k_4} a_{k_3}$$

where $\tilde{v}_{k_1 k_2 k_3 k_4}$is the antisymmetrized two body matrix elements

$$\begin{aligned} \tilde{v}_{k_1 k_2 k_3 k_4} &= \langle k_1 k_2 | \hat{v}(|k_3 k_4\rangle - |k_4 k_3\rangle) \\ &= \iint d^3\vec{r}_1 d^3\vec{r}_2 \phi^*_{k_1}(\vec{r}_1)\phi^*_{k_2}(\vec{r}_2) v(\vec{r}_1,\vec{r}_2) \left[\phi_{k_3}(\vec{r}_1)\phi_{k_4}(\vec{r}_2) - \phi_{k_3}(\vec{r}_2)\phi_{k_4}(\vec{r}_1)\right] \end{aligned}$$

This is a quite involved quantity and as it has four indexes the number of them required in typical calculations can be very large (billions of them!). Therefore, it is not surprising that, in order to alleviate the burden imposed by their calculation, simple analytical forms are chosen for the interaction and the basis wave functions. For instance, in the Gogny force the potential energy is parametrized in terms of gaussians and the basis is that of the harmonic oscillator whereas in the case of Skyrme like interactions, the potential energy is chosen to be zero range and therefore is proportional to Dirac's delta function or its derivatives. The efficient calculation of the two body matrix elements has become an art, specially in atomic physics and quantum chemistry.

A linear transformation among creation and annihilation operators is denoted "canonical" if it preserves the canonical commutation relations. In the Hartree-Fock case, where creation and annihilation operators are not mixed, the allowed transformations are of the kind

$$d^+_k = \sum_l D_{lk} a^+_l$$

and its hermitian conjugate. The requirement on the canonical commutation relation

$$\{d_k, d^+_{k'}\} = \sum_{ll'} D^*_{lk} D_{l'k'} \{a_l, a^+_{l'}\} = (D^+ D)_{kk'} = \delta_{kk'}$$

implies that the transformation matrix has to be unitary (that is, its hermitian conjugate is its inverse). The commutation relations for creation operators alone or annihilation operators are alone are straightforwardly satisfied. In terms of Hilbert space states, a canonical

transformation represents nothing but a linear combination of states

$$|\Psi_k\rangle = \sum_l D_{lk}|\varphi_l\rangle$$

that can also be portrayed as the decomposition of the state $|\Psi_k\rangle$ as a linear combination of set of states $|\varphi_l\rangle$.

Given an arbitrary unitary complex transformation D represented by an $N \times N$ matrix, the number of independent parameters is given by $2N^2 - N(N-1) - N = N^2$ where $2N^2$ is the number of independent parameters in a complex $N \times N$ matrix. The quantity $N(N-1) = 2 \times (N(N-1)/2)$ is the number of restrictions imposed by the upper triangle matrix in the condition $D^+D = \mathbb{I}$ (there are $N(N-1)/2$ elements in the upper triangle, each of them complex). Finally, the subtracting N is the number of conditions in the diagonal (which is a real number by construction). With those general creation operators d_k^+ we can construct the most general HF product state

$$|\Phi\rangle = \prod_{k=1}^{A} d_k^+|-\rangle$$

In all quantum mechanical calculations is convenient to refer all the abstract quantities to some kind of basis by means of linear transformations in such a way that the calculation is referred to the coefficients of the linear transformation instead of to the abstract quantities. With this in mind, we refer our mean field wave functions to some basis made of N creation operators a_l^+ $\{l = 1, \ldots, N\}$ that can generate $\begin{pmatrix} N \\ A \end{pmatrix}$ different Slater determinants of A particles.

To finish this section, we will discuss now how to evaluate mean values and overlaps between general A particle "independent particle" wave functions. First, let us focus in the evaluation of mean values of operators and consider the typical mean value

$$\langle\phi|d_k^+ d_l^+ d_m d_n|\phi\rangle$$

where

$$|\phi\rangle = \prod_{r=1}^{A} d_r^+|\rangle.$$

The key fact is that $|\phi\rangle$ is the vacuum of d_k^+ if k is included in the set of indexes entering the definition of $|\phi\rangle$, that is, the set $1, \ldots A$. This kind of indexes will be called "particle like" or

"particle" in the following. The state $|\phi\rangle$ is also the vacuum of d_m when m is not included in the set defining $|\phi\rangle$. This kind of indexes will be denoted "hole like" or "hole" in the following. It is easy to convince oneself about this fact by using the canonical commutation relations to move d_k^+ next to the left of the same creation operator in $|\phi\rangle$ and then use the property $\left(d_k^+\right)^2 = 0$ that is Pauli exclusion principle and is a consequence of the fermion commutation relations. For d_m we use the same commutation relations to jump over the creation operators in $|\phi\rangle$to reach the vacuum that is annihilated by d_m. Using hermitian conjugation, we can also show that $\langle\phi|d_k = 0$ if k is a "particle" index and $\langle\phi|d_l^+ = 0$ if l is a "hole" index. With this properties we can conclude that $\langle\phi|d_k^+ d_l^+ d_m d_n|\phi\rangle$ will only be different from zero if m, n, k and l are all of them "particle like". Assuming this to be the case we use the commutation relations to move the creation operators to the right

$$\begin{aligned}
\langle\phi|d_k^+ d_l^+ d_m d_n|\phi\rangle &= -\langle\phi|d_k^+ d_m d_l^+ d_n|\phi\rangle + \delta_{lm}\langle\phi|d_k^+ d_n|\phi\rangle \\
&= \langle\phi|d_k^+ d_m d_n d_l^+|\phi\rangle + \delta_{lm}\langle\phi|d_k^+ d_n|\phi\rangle - \delta_{ln}\langle\phi|d_k^+ d_m|\phi\rangle \\
&= \delta_{lm}\langle\phi|d_k^+ d_n|\phi\rangle - \delta_{ln}\langle\phi|d_k^+ d_m|\phi\rangle \\
&= \delta_{lm}\delta_{kn} - \delta_{ln}\delta_{km}
\end{aligned}$$

Let us now assume the existence of some creation operators f_k^+ , related to the $d_l^+$by a unitary transformation $f_k^+ = \sum_l F_{lk} d_l^+$. The mean value

$$\langle\phi|f_{k'}^+ f_{l'}^+ f_{m'} f_{n'}|\phi\rangle = \sum_{klmn} F_{kk'} F_{ll'} F_{mm'} F_{nn'} \langle\phi|d_k^+ d_l^+ d_m d_n|\phi\rangle$$

can be easily computed in terms of a quantity, usually denoted byρ and defined as

$$\rho_{m'k'} = \sum_{mk\in\text{particle}} F_{kk'} F_{mm'} \delta_{km}$$

The final result is

$$\langle\phi|f_{k'}^+ f_{l'}^+ f_{m'} f_{n'}|\phi\rangle = \rho_{n'k'}\rho_{m'l'} - \rho_{n'l'}\rho_{m'k'}$$

which is a particular case of the general Wick's theorem for the evaluation of mean values of an arbitrary number of creation and annihilation operators. Those mean values are given as the sum of the product of all possible contractions of two operators (the density)

$$\langle\phi|f_{k'}^+ f_{n'}|\phi\rangle = \rho_{n'k'}$$

The number of terms increases exponentially as the double factorial of the number of creation and annihilation operators in the mean value minus one (some of the terms may be zero as is the case in the present example. The extension to overlaps

$$\frac{\langle\phi|f^+_{k'}f^+_{l'}f_{m'}f_{n'}|\phi'\rangle}{\langle\phi|\phi'\rangle}$$

gives a similar result but in this case the contractions are given in terms of the overlap densities

$$\frac{\langle\phi|f^+_{k'}f_{n'}|\phi'\rangle}{\langle\phi|\phi'\rangle} = \overline{\rho}_{n'k'}$$

To finish this section let us mention that an equivalent result can also be shown not for mean values but for ensemble averages like the ones that appear naturally in the statistical description of ensemble averages (finite temperature systems).

III. THE HARTREE-FOCK METHOD (MEAN FIELD APPROXIMATION)

In the Hartree-Fock approximation it is assumed that the wave function of an A particle system can be approximated by an independent particle wave function

$$|\Phi\rangle = \prod_{k=1}^{A} d^+_k|-\rangle$$

where the d^+_k are creation operators to be specified later and $|-\rangle$ represents the wave function of the true vacuum. The energy associated to such wave function can be easily computed using the second quantization form of the hamiltonian

$$\hat{H} = \sum_{kl} t_{kl}a^+_k a_l + \frac{1}{4}\sum_{klmn}\tilde{v}_{klmn}a^+_k a^+_l a_n a_m$$

written in a given set of basis states associated to the creation and annihilation operators a^+_k and a_l (for instance a harmonic oscillator basis, or the set of eigenstates of the Wood-Saxon potential, or even plane waves as in the description of nuclear matter, etc). The energy associated to $|\Phi\rangle$ can be easily computed using Wick's theorem

$$E = \sum_{kl} t_{kl}\rho_{lk} + \frac{1}{4}\sum_{klmn}\tilde{v}_{klmn}(\rho_{mk}\rho_{nl} - \rho_{ml}\rho_{nk})$$

where the density matrix $\rho_{mk} = \sum_p D_{mp}D^*_{kp}$ is given in terms of the unitary transformation relating d^+_k with a^+_l, that is $d^+_k = \sum_l D_{lk}a^+_l$ and the index p in the sum refers to "particle

type", that is, all the orbitals d_p^+which are occupied in the product wave function $|\Phi\rangle$. The energy is a functional of the wave function $|\Phi\rangle$, through the dependence on the density matrix. Finally, the density matrix depends on the free parameters of the D transformation matrix. The coefficients in D are determined by invoking the variational principle on the energy, that is, the optimal D coefficients to represent the ground state of the system are those that minimize the energy

$$E[\rho + \delta\rho] - E[\rho] = \sum_{kl} \delta\rho_{kl} \frac{\partial E}{\partial \rho_{kl}} = \sum_{klmn} \delta D_{mn} \frac{\partial \rho_{kl}}{\partial D_{mn}} \frac{\partial E}{\partial \rho_{kl}} = 0.$$

The variation of the energy with respect to D has to be handled with care as not all of the D matrix elements are independent of each other. As previously mentioned, the matrix D is complex unitary $N \times N$ matrix with N^2 parameters (a $N \times N$ matrix with complex entries contains $2N^2$ parameters, but the unitary requirements $D^\dagger D = \mathbb{I}$ impose N^2constraints). Any unitary matrix can be parametrized as the exponential of an anti-hermitian matrix that is usually expressed as

$$D = e^{iZ}$$

in terms of a complex, hermitian, $N \times N$ matrix Z with N^2 free parameters (the same number as D, obviously !). The recipe to handle the free parameters in Z is to use hermiticity to convert any Z^*_{mk} into Z_{km} and consider all (no restriction in the indexes) the Z_{mk} as free parameters. With this recipe in mind, we write

$$\rho = DFD^+ = e^{iZ} F e^{-iZ}$$

where F is a diagonal matrix with ones in the first A entries of the diagonal (occupied particles) and zeros elsewhere (the density matrix in the Hartree-Fock basis D !). With this parametrization of the density we have $\delta\rho = i(\delta Z \rho - \rho \delta Z)$. Introducing the Hartree-Fock hamiltonian

$$h_{mn} = \frac{\partial E}{\partial \rho_{mn}}$$

the minimum condition becomes

$$i\mathrm{Tr}[\delta Z [h, \rho]] = 0$$

which is valid for arbitrary δZ what implies

$$[h, \rho] = 0$$

which is the final form of the Hartree-Fock equation. In the Hartree- Fock basis D the HF equation takes the form

$$\overline{h}F - F\overline{h} = 0$$

where $\overline{h} = D^{+}hD$. Taking into account that $(1-F)F = 0$ the above condition becomes

$$(1-F)\overline{h}F = F\overline{h}(1-F) = 0$$

For any matrix M in the HF basis the product $FM(1-F)$ is denoted as the particle-hole part of the matrix M. Therefore, the HF condition is expressed as the requirement that the HF hamiltonian in the HF basis must have vanishing particle-hole (and hole-particle) matrix elements. Obviously this condition is fully satisfied if $\overline{h}$ is diagonal and usually the HF equation is recast as the non-linear eigenvalue problem

$$hD = D\epsilon$$

where the non-linearity comes from the dependence of h on ρ that implies a dependence on D. The entries of the diagonal matrix of eigenvalues ϵ are referred to as the "single particle energies".

The non-linearity of the HF equation has as a consequence the possibility of spontaneous symmetry breaking of the HF solution. That means that if the interaction v is invariant under some kind of symmetry (rotational invariance, translational invariance, parity, etc) the solution of the HF equation does not necessarily have to preserved those symmetries. As a consequence of the spontaneous symmetry breaking mechanism the HF spatial density can break rotational invariance (deformed intrinsic states), translational invariance (localized nuclei), parity (reflection asymmetric shapes), etc. This mechanism allows to incorporate many correlations into a simple product wave function and can be understood in terms of variational arguments. Let us assume a system with a single particle basis made of wave functions eigenstates of the angular momentum a^{+}_{nljm}. The only possibility within a pure mean field framework to get a 0^{+} state (to describe the ground state of an even-even nucleus) is to occupy the j orbital with $2j+1$ particles. The wave function is fully determined by the symmetry requirements and there is no freedom, in the form of variational parameters, to seek for a configuration producing a lower energy. Another possibility, slightly outside the mean field framework , is to consider a convenient statistical admixture of states like in

the two particle case

$$|0^+\rangle = \sum_m \frac{(-)^m}{2j+1} a^+_{nljm} a^+_{nlj-m} |-\rangle$$

Again the symmetry requirements of the 0^+quantum numbers fix the weights of the allowed linear combinations. On the other hand, if symmetry breaking is allowed, general linear combinations of the kind $d^+_q = \sum_{nljm} D_{nljm,q} a^+_{nljm}$ are allowed which brings in many free variational parameters that can, conveniently chosen, lower the energy of the systems if the nuclear interactions permits. It turns out that the nuclear interaction favors in many cases the breaking of symmetries being the rotational and translational invariance the two most popular regarding spatial symmetries.

IV. THE LIPKIN MODEL AS AN EXAMPLE

Over the years the Lipkin-Meshkov-Glick (LMG) model has been used as a paradigm of solvable model to test many-body theories and approximations, see Ref [12] for a detailed account of this model and its use in Nuclear Physics. It has also been used to model the transition to "deformed" systems by studying the behavior of the mean field solution as a function of the two-body-force strength. Here we will use another viewpoint [13] that assigns one of the LMG model parameter the meaning of a reflection symmetry breaking parameter (octupole deformation). In this way the Lipkin model is used to study the transition to a parity-mixed system with the aim of understanding the features of low-lying levels associated to the octupole degree of freedom. The reason is that in this framework we can also use the model to go beyond the mean field and restore symmetries (parity in this case) as well as considering long range correlations by means of the generator coordinate method.

The LMG model is composed of a N-fermion system with two energy levels, each having an N-fold degeneracy (half filling). Each state in the model is described by two quantum numbers p and σ. The quantum number p can take N possible values and it is used to distinguish levels in each of the N-fold-degenerated shells. The label σ can take two values: $+1$ if the particle is in the upper shell and -1 if it is in the lower one. The particles interact via a monopole-monopole interaction which only scatters particles between upper and lower states having the same value of p. The model is described by the hamiltonian

$$H = \frac{1}{2}\epsilon \sum_{p,\sigma} \sigma a^+_{p\sigma} a_{p\sigma} + \frac{1}{2} V \sum_{p,p'\sigma} a^+_{p\sigma} a^+_{p'\sigma} a_{p'-\sigma} a_{p-\sigma} \tag{1}$$

where $a^+_{p\sigma}$ and $a_{p\sigma}$ are creation and destruction operators, respectively, of a state with quantum numbers p and σ. The operators in the interaction term can be reordered to express it in the following form

$$\frac{1}{2}V\sum_{p,p'\sigma} a^+_{p\sigma}a_{p-\sigma}a^+_{p'\sigma}a_{p'-\sigma}$$

which clearly shows the operator $a^+_{p\sigma}a_{p-\sigma}$ responsible of destroying a particle with quantum numbers $p-\sigma$ and creating another one in $p\sigma$. This is process we alluded to previously as "scattering of particles between lower and upper shells". Introducing the so-called "quasi-spin operators"

$$\hat{K}_0 = \frac{1}{2}\sum_{p,\sigma}\sigma a^+_{p\sigma}a_{p\sigma} \qquad \hat{K}_+ = \sum_p a^+_{p+}a_{p-} \qquad \hat{K}_- = (\hat{K}_+)^+ \tag{2}$$

that satisfy the same kind of commutation relations as the three components of the angular momentum operators J_z, $J_\pm$ the Hamiltonian can be written in a more compact form that is more amenable to the technology of group theory

$$\hat{H} = \epsilon\hat{K}_0 - \frac{1}{2}V(\hat{K}_+\hat{K}_+ + \hat{K}_-\hat{K}_-). \tag{3}$$

The mean field solution of the model is easily obtained by minimization of the mean field value of the energy. To compute the mean field energy an expression of the most general Slater determinant in the model is needed. The hamiltonian of the model is invariant under a permutation of the N levels below and the corresponding levels above the Fermi surface. Therefore, the solutions of the model will be restricted to those solutions completely symmetric under such permutation. Under the previous restriction, the most general unnormalized Slater determinant is given by (see the Thouless theorem below)

$$|z\rangle = \exp(z\hat{K}_+)|0\rangle \tag{4}$$

where z is a complex number and $|0\rangle$ is the unperturbed vacuum obtained by filling up the lowest N orbits with energy $-\epsilon/2$

$$|0\rangle = \prod_{p=1}^{N} a^+_{p-}|-\rangle.$$

Using the commutation rules of fermion operators it is easy to show that $[\hat{K}_+, a^+_{p-}] = a^+_{p+}$ and $[\hat{K}_+, a^+_{p+}] = 0$. These two results allow to obtain

$$\begin{aligned}\exp(z\hat{K}_+)a^+_{p-}\exp(-z\hat{K}_+) &= a^+_{p-} + za^+_{p+}\\ \exp(z\hat{K}_+)a^+_{p+}\exp(-z\hat{K}_+) &= a^+_{p+} - z^*a^+_{p-}\end{aligned}$$

that lead to the definition of a new set of operators

$$\begin{aligned} d_{0p} &= D \ \left(a^+_{p-} + z a^+_{p+}\right) \\ d^+_{1p} &= D'^* \ \left(a^+_{p+} - z^* a^+_{p-}\right) \end{aligned}$$

and the corresponding hermitian conjugated d^+_{0p} and d_{1p} which are defined in terms of two parameters D and D' that are introduced to insure that the new set of operators satisfy canonical commutation relations. A little algebra shows that $|D| = |D'| = (1+|z|^2)^{-1/2}$ implying that the transformation

$$\begin{pmatrix} d_{0p} \\ d^+_{1p} \end{pmatrix} = \begin{pmatrix} D_{-0} & D_{+0} \\ D_{-1} & D_{+1} \end{pmatrix} \begin{pmatrix} a^+_{p-} \\ a^+_{p+} \end{pmatrix}$$

with

$$\begin{aligned} D_{-0} &= (1+|z|^2)^{-1/2} \\ D_{+0} &= z(1+|z|^2)^{-1/2} \\ D_{-1} &= -z^*(1+|z|^2)^{-1/2} \\ D_{+1} &= (1+|z|^2)^{-1/2} \end{aligned}$$

is a unitary transformation. It is customary to introduce a change of variables to simplify the notation $D_{-0} = \cos\alpha$ and $D_{+0} = \sin\alpha e^{i\varphi}$. With the new variables we write

$$\begin{pmatrix} d_{0p} \\ d^+_{1p} \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha e^{i\varphi} \\ \sin\alpha e^{-i\varphi} & \cos\alpha \end{pmatrix} \begin{pmatrix} a^+_{p-} \\ a^+_{p+} \end{pmatrix}$$

and its inverse

$$\begin{pmatrix} a^+_{p-} \\ a^+_{p+} \end{pmatrix} = \begin{pmatrix} \cos\alpha & \sin\alpha e^{i\varphi} \\ \sin\alpha e^{-i\varphi} & \cos\alpha \end{pmatrix} \begin{pmatrix} d_{0p} \\ d^+_{1p} \end{pmatrix}$$

A more relaxed look at the previous expressions reveals that the unitary transformation is mixing creation and annihilation operators d_{0p} and d^+_{1p} with no apparent reason. However, behind this choice there is the desire to simplify the notation in the following respect: with the traditional assignment the initial vacuum $|0\rangle$ is the vacuum of a^+_{p-} (the Pauli exclusion principle prevents to create a particle in an already occupied level) and also of a_{p+} (it is not possible to destroy a non-existing particle). With the transformation as written the new HF

wave function $|\phi(\alpha,\varphi)\rangle = \prod_{p=1}^{N} d_{0p}|-\rangle$ will be the vacuum of d_{0p} and d_{1p}. The parameters of the transformation α and φ are determined by the HF equation. In order to compute all the required quantities we have to compute the different contractions

$$\begin{aligned}
\langle\phi(\alpha,\varphi)|a^+_{m+}a_{m+}|\phi(\alpha,\varphi)\rangle &= D^*_{+0}D_{+0} = \sin^2\alpha \\
\langle\phi(\alpha,\varphi)|a^+_{m+}a_{m-}|\phi(\alpha,\varphi)\rangle &= D^*_{+0}D_{-0} = \sin\alpha\cos\alpha e^{-i\varphi} \\
\langle\phi(\alpha,\varphi)|a^+_{m-}a_{m+}|\phi(\alpha,\varphi)\rangle &= D^*_{-0}D_{+0} = \sin\alpha\cos\alpha e^{i\varphi} \\
\langle\phi(\alpha,\varphi)|a^+_{m-}a_{m+}|\phi(\alpha,\varphi)\rangle &= D^*_{-0}D_{-0} = \cos^2\alpha
\end{aligned}$$

The mean values of observables are easily computed

$$\begin{aligned}
\langle\phi(\alpha,\varphi)|\hat{K}_0|\phi(\alpha,\varphi)\rangle &= \frac{N}{2}(\sin^2\alpha - \cos^2\alpha) \\
\langle\phi(\alpha,\varphi)|\hat{K}_+\hat{K}_+|\phi(\alpha,\varphi)\rangle &= N(N-1)\sin^2\alpha\cos^2\alpha e^{-2i\varphi}
\end{aligned}$$

and with them the mean value of the hamiltonian

$$\langle\phi(\alpha,\varphi)|\hat{H}|\phi(\alpha,\varphi)\rangle = -\frac{\epsilon N}{2}(\cos(2\alpha) + \frac{\kappa}{2}\sin^2(2\alpha)\cos(2\varphi))$$

given in terms of $\kappa = (N-1)V/\epsilon$. Instead of showing a plot of the energy as a function of the two variational parameters we give in Fig 1 the Python code required to create such a plot easily in a standard Linux distribution. The reader is encouraged to type in and run the code with different choices of the parameters.

Instead of solving the HF equation we will proceed to minimize the energy as a function of the two parameters α and φ. It turns out that the lowest energy solution corresponds to $\varphi = 0$ and therefore the minimization is for a simple one dimensional function. The mean field energy as a function of the variational parameter φ can be written as

$$\langle\alpha|\hat{H}|\alpha\rangle = -\frac{\epsilon N}{2}\left(\cos(2\alpha) + \frac{\kappa}{2}\sin^2(2\alpha)\right) \tag{5}$$

where κ is a function of the interaction strength V and the single particle energy spacing ϵ, i.e. : $\kappa = \frac{(N-1)V}{\epsilon}$.

In Fig 2 the mean field energy is depicted as a function of α for different values of κ. For $\kappa < 1$ a single minimum located at $\alpha = 0$ is observed while for $\kappa > 1$ a characteristic two-well structure appears with the minima located at $\alpha = \pm\frac{1}{2}\arccos(\frac{1}{\kappa})$ (mean field solution). The $\alpha \neq 0$ Slater determinant is interpreted as a “deformed" wave function and the transition at $\kappa = 1$ is referred as a transition to a “deformed" system.

```
from pylab import *

def H(a,f): return -e*omeg/2 * (np.cos(2*a)+0.5*ka*np.sin(2*a)**2*cos(2*f))

n = 256
a = np.linspace(0,3.1415,n)
f = np.linspace(0,3.1415,n)
X,Y = np.meshgrid(a,f)

axes([0.025,0.025,0.95,0.95])

# ----------------------------------------------------
#                    Lipkin model parameters
# ----------------------------------------------------
e=1
omeg=15
ka=2.5
# ----------------------------------------------------

contourf(X, Y, H(X,Y), 8, alpha=.75, cmap=cm.hot)
C = contour(X, Y, H(X,Y), 8, colors='black', linewidth=.5)
clabel(C, inline=1, fontsize=10)

xticks([]), yticks([])
# savefig('../figures/contour_ex.png',dpi=48)
show()
```

Figure 1: Python code to plot the Lipkin's model energy as a function of the variational parameters α and φ.

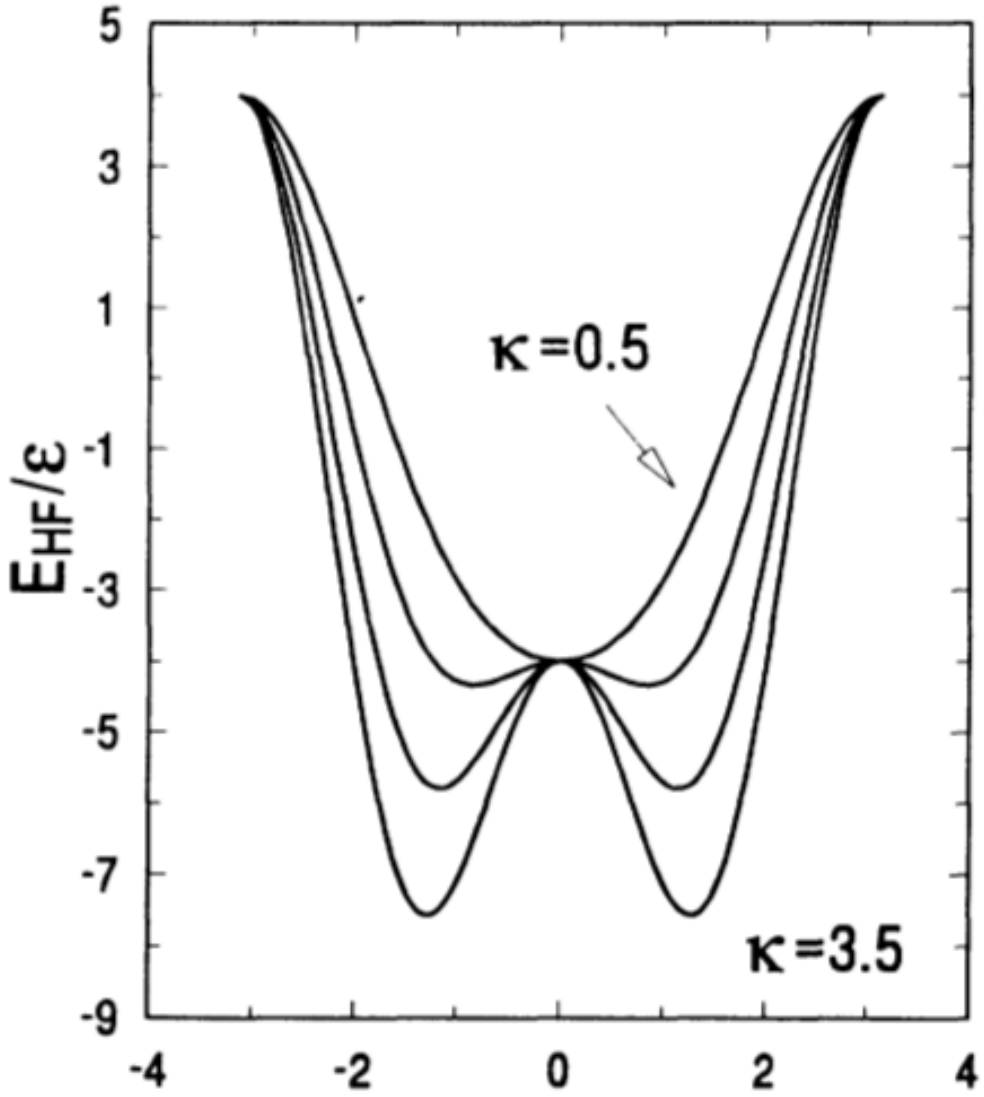

Figure 2: The HF energy of the Lipkin model as a function of α and for differente values of the parameter κ. For $\kappa = 1$ a transition from a regime with a single minimum at $\alpha = 0$ to another with two minima is clearly observed.

To connect the deformed mean field wave function with a parity-breaking Slater determinant the parity quantum number has to be assigned to any of the quantum numbers of the model. The easiest way to obtain a parity-breaking $|\alpha\rangle$ is to have a negative parity $\hat{K}_+$ operator (see Eq. (4)). The $\hat{K}_+$ operator connects states with the same quantum number p but belonging to different σ shells. By assigning given parities to the p, $\sigma = +1$ states and the opposite to the corresponding state p, $\sigma = -1$ a negative parity $\hat{K}_+$ operator is obtained. A simpler assignment is to identify σ as the parity quantum number. In the calculations

that follow this assignment is equivalent up to a phase to the former and I will use it in the following.

Once the parity quantum number has been assigned one can wonder how well the two shells LMG model can describe the physics of octupole deformation. The onset of octupole deformed shapes is associated with the coupling of the intruder sub-shell (l, j) and the nearby normal parity sub-shell (l -3, j -3). The regions of nuclei with strong octupole correlations correspond to particle numbers around 34 ($g_{9/2}$ $p_{3/2}$ coupling), 56 ($h_{11/2}$ $d_{5/2}$ coupling), 88 ($i_{13/2}$ $f_{7/2}$ coupling) and 134 ($j_{15/2}$ $g_{9/2}$ coupling), i.e. the tendency toward octupole deformation occurs just above closed shells. Therefore, it is reasonable to think that the physics of octupole deformation is almost contained in the coupling of the (l, j) and (l - 3, j - 3) sub-shells. In the study of the octupole degree of freedom the neglecting of non-axial effects is a reasonable assumption and, therefore, only the coupling between states with the same j_z is allowed. In this instance, the (l, j) and (l - 3, j - 3) coupling can be modeled by two shells of opposite parity and the same number of particles in each sub-shell, where a particle in one shell can only be scattered to a state in the other shell having the same quantum numbers of the original state. This is the physical situation described by the Lipkin model.

Although the "monopole-monopole" two-body interaction of the LMG model can hardly contain the richness of the full two-body interaction part involved in the appearance of octupole deformation effects, the results of the model at the mean field level compare qualitatively well with calculations carried out in more realistic cases [13]. In such realistic calculations, a constrained HFB calculation was carried out using the octupole operator as constraint. The HFB energy plotted as a function of the mean value of the constraint ($q_3 = \langle \hat{Q}_{30} \rangle$) shows the characteristic two-well structure and $q_3 \rightarrow -q_3$ degeneracy seen in the LMG model. By redefining the α scale Fig 2 could correspond to any of the energy curves of those realistic cases. This qualitative agreement at the mean field level gives confidence in the use of the LMG hamiltonian as a model suited to describe the gross features of octupole deformed systems.

V. PAIRING CORRELATIONS, THE BCS AND THE HARTREE- FOCK- BOGOLIUBOV METHOD

In order to describe the short range correlations that lead to the phenomenon of superfluidity in the atomic nucleus in a mean field scheme a generalization of the HF method is required. Instead of the unitary transformation of Eq introduced in the HF case one is forced to introduce quasiparticle creation and annihilation operators which are linear combinations of both creation and annihilation single particle operator. The mixing of creation and annihilation operators is a clear indication that the transformation can break the particle number symmetry and therefore a product wave function built from those quasiparticle operators will not be an eigenstate of the number of particles operator. We will start our theoretical description by introduction the BCS method developed originally to describe superconductivity and soon after applied in nuclear physics to explain a wealth of experimental data. The idea of the BCS method is to consider canonical transformations of the form

$$\begin{aligned} \alpha_k &= u_k c_k + v_k c_{\overline{k}}^+ \\ \alpha_{\overline{k}} &= u_k c_{\overline{k}} - v_k c_k^+ \end{aligned}$$

where $\overline{k}$ denotes the time reserved of the quantum number k. The parameters u_k and $v_k$are not free as they have to satisfy the constraint $u_k^2 + v_k^2 = 1$. The corresponding wave function is defined as the vacuum of the annihilation operators

$$|BCS\rangle = \mathcal{N} \prod_k \alpha_k |-\rangle = \prod_{k>0} (u_k + v_k c_k^+ c_{\overline{k}}^+)|-\rangle$$

The mean value of the number of particles with quantum number k operator is given by

$$\langle BCS|c_k^+ c_k|BCS\rangle = v_k^2.$$

This result allows to interpret the parameters v_k^2 as the occupancy of the orbital k. The theory developed so far is invariant under time reversal by construction and therefore is only suited to describe nuclei with an even number of protons and neutrons. The extension to odd-A systems will be discussed below. It is also clear from the structure of the BCS wave function that it breaks the number of particles symmetries as can be shown by looking at its structure for a four particle system

$$|BCS\rangle = u_1 u_2 + u_1 v_2 c_2^+ c_{\overline{2}}^+ |-\rangle + (1 \Leftrightarrow 2) + u_1 v_2 u_2 v_1 c_1^+ c_{\overline{1}}^+ c_2^+ c_{\overline{2}}^+ |-\rangle.$$

It is clearly seen that the BCS wave function is a linear combination of states with 0, 2 and 4 particles. We also notice that states with an odd number of particles cannot enter into the BCS wave function as written. This fact is expressed by saying that the BCS wave function preserves the "number parity" symmetry (if the number of particles in the linear combinations are even or odd numbers). The wave function just described is said to have even "number parity". To describe odd-A systems we need wave functions with odd number parity and therefore an extension of BCS (blocked BCS) is required to treat those systems. The generalization of BCS to allow at the same time transformations among the single particle creation and annihilation operators gives rise to the celebrated Hartree- Fock-Bogoliubov (HFB) method.

In the standard HFB method [**?**] quasi-particle operators β_μ^+ are introduced as linear combinations of the creation and annihilation single particle operators corresponding to an arbitrarily chosen (usually a Harmonic oscillator) basis

$$\beta_\mu^+ = \sum_m U_{m\mu} c_m^+ + V_{m\mu} c_m. \tag{6}$$

The HFB ground state wave function is defined by the condition of being the vacuum of all the quasi-particle annihilation operators, that is $\beta_\mu|\phi\rangle = 0$. A more concise definition is given by $|\phi\rangle = \prod_\mu \beta_\mu|0\rangle$ where the index μ run over all the quasi-particle annihilation operators that do not annihilate the true vacuum $|0\rangle$. The previous results will describe the ground state of an even-even nucleus as it can be shown that a paired HFB wave function is a linear combination of product wave functions with an even number of particles. On the other hand, odd-particle systems are handled by the "blocked" HFB wave functions

$$|\tilde{\phi}\rangle_{\mu_B} = \beta_{\mu_B}^+|\phi\rangle \tag{7}$$

where μ_B is any of the quasi-particle indexes compatible with the symmetries of the odd-particle system as, for instance, the K quantum number or the parity. The Bogoliubov transformations in conveniently written in matrix form

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^+ & V^+ \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \equiv W^+ \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \tag{8}$$

that introduces the matrix W. To simplify even further the notation it is common to introduce

the set of quasiparticle operators

$$\alpha_\mu = \begin{cases} \beta_\mu & \mu = 1, \ldots, M \\ \beta^+_{\mu-M} & \mu = M+1, \ldots, 2M \end{cases}$$

$$\alpha_\mu = (\beta_1, \ldots, \beta_M, \beta^+_1, \ldots, \beta^+_M)$$

as well as the corresponding single particle operators

$$a \equiv (c, c^\dagger).$$

With the compact notation the Bogoliubov transformation of Eq (6) is written as

$$\alpha = W^\dagger a$$

The Bogoliubov transformation is a canonical transformation that preserves the canonical commutation relations (written in compact notation)

$$\{a_\mu, a_\nu\} = \sigma_{\mu\nu} = \begin{pmatrix} 0 & \mathbb{I} \\ \mathbb{I} & 0 \end{pmatrix}.$$

This condition imposes the condition $W^\dagger \sigma W = \sigma$ on the Bogoliubov transformation matrix. This condition implies that the matrix W is similar to a matrix of the group SO(N) matrix. The HFB wave function $|HFB\rangle$is built by requiring it to be the vacuum of the annihilation operators β_μ, that is $\beta_\mu |HFB\rangle = 0$. The connection between the HFB and the BCS methods is given by the Bloch-Messiah theorem that states that the W transformation can be decomposed as the product of three successive transformations

$$W = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix}$$

the D and C transformations correspond to unitary transformations. The D transformation transforms the original single particle basis in the **canonical basis** $c \to a$ (to be characterized in a more transparent way below). On the other hand, the C transformation represents an often irrelevant transformation among quasi-particles and finally $\bar{U}$, $\bar{V}$ are the

block-diagonal matrices

$$\overline{U} = \begin{pmatrix} 0 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 0 & & & & & & & & \\ & & & u_1 & 0 & & & & & & \\ & & & 0 & u_1 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & u_N & & & & \\ & & & & & & & u_N & & & \\ & & & & & & & & 1 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & 1 \end{pmatrix}$$

$$\bar{V} = \begin{pmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ & & & 0 & v_1 & & & & & & \\ & & & -v_1 & 0 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 0 & v_N & & & \\ & & & & & & -v_N & 0 & & & \\ & & & & & & & & 0 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & 0 \end{pmatrix}$$

that implement the BCS transformation among the single particle states of the canonical basis.

Once the Bogoliubov transformation is defined we have to find the way to compute mean values of operators. The task is simplified by the introduction of the "generalized density matrix"

$$\mathcal{R} = \langle a^\dagger a \rangle = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & 1-\rho^\dagger \end{pmatrix}$$

The different blocks entering the definition of $\mathcal{R}$ correspond to the density matrix $\rho_{mm'} = \langle\phi|\, c^\dagger_{m'} c_m \,|\phi\rangle = V^* V^T$ and the pairing tensor $\kappa_{mm'} = \langle\phi|\, c_{m'} c_m \,|\phi\rangle = V^* U^T$. The density

matrix ρ is the analogous of the density matrix in the HF theory whereas the pairing tensor is a quantity directly related to the existence of pairing correlations and is zero in the HF case (as it should be, because in the particle number preserving HF case it corresponds to the mean value of an operator not preserving particle number). It is not difficult to prove that the density matrix ρ is diagonal in the canonical basis and κ acquires a simple block structure where each of the blocks have the form

$$\begin{pmatrix} 0 & v_k \\ -v_k & 0 \end{pmatrix}.$$

For subsequent developments it is interesting to introduce the quasiparticle density matrix

$$\mathbb{R}_{\mu\nu} = \langle \alpha^\dagger_\mu \alpha_\nu \rangle = \begin{pmatrix} \langle \beta^\dagger_m \beta_\nu \rangle & \langle \beta_m \beta_\nu \rangle \\ \langle \beta^\dagger_m \beta^\dagger_\nu \rangle & \langle \beta_m \beta^\dagger_\nu \rangle \end{pmatrix}$$

which is connected to the particle density matrix by the Bogoliubov transformation

$$\mathcal{R} = W \mathbb{R} W^\dagger.$$

The quasiparticle density matrix has a diagonal structure in the simple case where the M diagonal elements are zero and the remaining M are one

$$\mathbb{R} = \begin{pmatrix} 0 & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

as can be easily proved by taking into account that the HFB wave function is the vacuum of the quasiparticle annihilation operators as well as the commutation relations for the quasiparticle operators. For blocked HFB wave functions $|\phi_i\rangle = \beta^+_i |\phi\rangle$ used to treat odd-A systems the quasiparticle density matrix is given by

$$\mathbb{R}_i = \begin{pmatrix} \mathbb{I}_i & 0 \\ 0 & \mathbb{I} - \mathbb{I}_i \end{pmatrix}$$

where the index i is that of the "blocked level" and the matrix $\mathbb{I}_i$ is a matrix with all its elements equal to zero except the "i"-th element in the diagonal which is one. Finally, the quasiparticle density matrix of a statistical collection of HFB excitations like the one that describes a macro-canonical system in equilibrium at temperature T is given by

$$\mathbb{R}_T = \begin{pmatrix} f & 0 \\ 0 & 1 - f \end{pmatrix}$$

In such a system the mean values have to be replaced by the statistical average represented by the trace of a given statistical operator D. The advantage of the general formalism to be developed below is that it is equally valid for the three cases what allows to develop the general HFB theory in an unified way.

The Bogoliubov coefficients are determined by the dynamics of the system by invoking the variational principle on the energy. The energy can be computed using the generalization of Wick's theorem to quasi-particles involving contractions that are given by the density matrix and pairing tensor described above. In the process of writing the energy is convenient to introduce the HF hamiltonian h and the pairing field Δ defined by

$$\begin{aligned} h_{ll'} &= \langle\phi| \left\{ \left[c_l, \hat{H} \right], c_{l'}^\dagger \right\} |\phi\rangle \\ \Delta_{ll'} &= \langle\phi| \left\{ \left[c_l, \hat{H} \right], c_{l'} \right\} |\phi\rangle \end{aligned}$$

and given in terms of the two body interaction matrix elements $\overline{v}_{ll'mm'}$ and the density matrix and pairing tensor by

$$\begin{aligned} \Gamma_{ll'} &= \sum_{qq'} \overline{v}_{lq'l'q}\ \rho_{qq'} \\ \Delta_{ll'} &= \frac{1}{2} \sum_{qq'} \overline{v}_{ll'qq'}\ \kappa_{qq'} \end{aligned}$$

The HF potential Γ is just the HF hamiltonian without the kinetic energy $h = t + \Gamma$. Finally the mean value of the Hamiltonian is given by the trace of all the involved matrices

$$\langle H \rangle = \mathrm{Tr}(t\rho) + \frac{1}{2}\mathrm{Tr}(\Gamma\rho) - \frac{1}{2}\mathrm{Tr}(\Delta\kappa^*)$$

In order to introduce into the formalism the density matrix $\mathcal{R}$ it is convenient to define the associated "hamiltonian matrix"

$$\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$$

and the kinetic energy

$$\mathcal{T} = \begin{pmatrix} t & 0 \\ 0 & -t^* \end{pmatrix}$$

to write

$$\langle H \rangle = \frac{1}{4}\mathrm{Tr}\left[\left(\mathcal{H} + \mathcal{T} \right) \mathcal{S} \right]$$

where

$$\mathcal{S} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & -\rho^* \end{pmatrix} = \mathcal{R} - \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

A useful property to be used later is

$$\mathrm{Tr}\left[(\mathcal{H}_1 - \mathcal{T})\,\mathcal{S}_2\right] = \mathrm{Tr}\left[(\mathcal{H}_2 - \mathcal{T})\,\mathcal{S}_1\right] \tag{9}$$

where $\mathcal{H}_1$ and $\mathcal{H}_2$ represent the hamiltonian matrices computed with the densities in $\mathcal{S}_1$ and $\mathcal{S}_2$. Once established that the energy is a functional of the density we have to express the variations of the density in term of the correct variational parameters. To this end we will use the generalized Thouless theorem: given an HFB wave function $|\phi\rangle$ with Bogoliubov amplitudes W, we can obtain another HFB wave function $|\phi'\rangle$, by means of the exponential of a general hermitian one body operator

$$|\phi'\rangle = e^{i\hat{Z}}\,|\phi\rangle$$

and

$$\hat{Z} = Z^0 + \frac{1}{2}Tr\left[Z^{11}\right] + \frac{1}{2}\sum_{\mu\nu}\mathbb{Z}_{\mu\nu}\alpha^\dagger_\mu\alpha_\nu$$

The hermitian matrix $\mathbb{Z}$ has the traditional block structure

$$\mathbb{Z} = \begin{pmatrix} Z^{11} & Z^{20} \\ -Z^{20*} & -Z^{11*} \end{pmatrix}$$

where Z^{11} and Z^{20} are hermitian and skew-symmetric respectively. When acting on a set of quasiparticle operators $\alpha = W^\dagger a$ with amplitudes $W(0)$, the exponential operator produces another set of quasiparticle operators $\alpha' = W^\dagger(Z)a$ with amplitudes $W(Z)$

$$\alpha' = e^{i\hat{Z}}\alpha e^{-i\hat{Z}} = W^\dagger(Z)a$$

The new Bogoliubov amplitudes are related to the original ones by

$$W(Z) = W(0)e^{i\mathbb{Z}}$$

By construction the new set $W(Z)$ satisfy the requirement to be a canonical transformation. The density matrix $\mathcal{R}(Z) = \langle\phi'|a^+a|\phi\rangle$is a function of the parameters of the $\mathbb{Z}$ matrix $\mathcal{R}(\mathbb{Z}) = W(\mathbb{Z})\mathbb{R}W^\dagger(\mathbb{Z}) = W(0)e^{i\mathbb{Z}}\mathbb{R}e^{-i\mathbb{Z}}W^\dagger(0)$ and therefore the variation of the density

$\delta\mathcal{R} = \mathcal{R}(Z) - \mathcal{R}(0)$ is simply given by $\delta\mathcal{R} = W(0)\left(e^{i\mathbb{Z}}\mathbb{R}e^{-i\mathbb{Z}} - \mathbb{R}\right)W^\dagger(0)$. Expanding in a power series the exponential we arrive after some algebra to

$$\delta\mathcal{R} = \delta\mathcal{R}^{(1)} + \delta\mathcal{R}^{(2)} + \ldots = W(0)\left[i\left[\mathbb{Z},\mathbb{R}\right] - \frac{1}{2}\left[\mathbb{Z},\left[\mathbb{Z},\mathbb{R}\right]\right] + \ldots\right]W^\dagger(0).$$

From here it is easy to guess the n-th term

$$\delta\mathcal{R}^{(n)} = W(0)\left[\frac{i^n}{n!}\left[\mathbb{Z},\left[\cdots\left[\mathbb{Z},\mathbb{R}\right]\right]\right] + \ldots\right]W^\dagger(0)$$

The matrix $\mathcal{S}$ entering the expression of the energy can be expanded accordingly and it turns out that $\delta\mathcal{S}^{(n)} = \delta\mathcal{R}^{(n)}$. We are now in the position of computing the variation of the HFB energy to establish the HFB equations. The HFB energy is given by

$$\langle\phi'|H|\phi'\rangle(Z) = \frac{1}{4}\mathrm{Tr}\left[\left(\mathcal{H}(Z) + \mathcal{T}\right)\mathcal{S}(Z)\right] \tag{10}$$

At this point it is convenient to write the block hamiltonian matrix in compact form

$$\mathcal{H}_{\mu\nu}(Z) = \mathcal{T}_{\mu\nu} + \frac{1}{2}\sum_{\rho\sigma}\mathcal{W}_{\mu\nu\rho\sigma}\mathcal{R}_{\sigma\rho}(Z) = \mathcal{H}_{\mu\nu}(0) + \delta\mathcal{H}_{\mu\nu} \tag{11}$$

where the generalized interaction matrix elements $\mathcal{W}_{\mu\nu\rho\sigma}$ have been introduced. We will not need the explicit form of $\mathcal{W}$ for the derivation of the HFB equation and they are only required to study the stability matrix of the HFB or the Randon Phase Approximation (RPA) matrix. The variation of the energy is then given up to first order in Z by

$$\delta E = \langle H\rangle(Z) - \langle H\rangle(0) = \frac{1}{4}\mathrm{Tr}[\delta\mathcal{H}^{(1)}\mathcal{S} + (\mathcal{H} + \mathcal{T})\delta\mathcal{S}^{(1)}] + \cdots$$

Using the property of Eq (9) we can write $\mathrm{Tr}\left[\delta\mathcal{H}\mathcal{S}\right] = \mathrm{Tr}\left[\left(\mathcal{H} - \mathcal{T}\right)\delta\mathcal{S}\right]$ and from here $\delta E = \frac{1}{2}\mathrm{Tr}[\mathcal{H}\delta\mathcal{S}^{(1)}] + \cdots$. Using the explicit expression of the first order variation of $\mathcal{S}$, $\delta S^{(1)} = iW(0)\left[\mathbb{Z},\mathbb{R}\right]W^\dagger(0)$ we finally arrive to the variation of the HFB energy with respect to the Z parameters

$$\delta E = \frac{i}{2}\left[\mathbb{R},\mathbb{H}\right] : \mathbb{Z} + \cdots$$

where some new notation has been introduced. First the scalar product : defined as

$$A : B = \frac{1}{2}\mathrm{Tr}(AB) = \frac{1}{2}\sum_{\mu\nu}A_{\mu\nu}B_{\nu\mu}$$

and second the hamiltonian matrix in the quasiparticle basis

$$\mathbb{H} = W^{\dagger}(0)\mathcal{H}W(0) = \begin{pmatrix} H^{11} & H^{20} \\ -H^{20*} & -H^{11*} \end{pmatrix}.$$

The HFB equation corresponds to the requirement that the variation of the energy with respect to the variational parameters Z to be zero, that is

$$[\mathbb{R}, \mathbb{H}] = 0 \tag{12}$$

Obviously, this equation is invariant under similarity transformations and therefore is fully equivalent to

$$[\mathcal{R}, \mathcal{H}] = 0 \tag{13}$$

that is the more traditional HFB equation. Eq. (12) is satisfied if $\mathbb{H}$ becomes a diagonal matrix denoted E. Due to the block structure of this matrix the eigenvalues come in pairs with one of the members minus the other

$$E = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}$$

Finally, the HFB equation is equivalent to the non-linear algebraic eigenvalue problem

$$\mathcal{H}W(0) = W(0)E$$

which is similar in structure to the HF equation. This is a non-linear equation because the matrix to be diagonalized $\mathcal{H}$ depends on the eigenvectors W through the density matrix $\mathcal{R}$. The standard method of solution is to guess some initial density matrix $\mathcal{R}^{(0)}$, with that density the hamiltonian matrix $\mathcal{H}^{(0)}$ is computed and diagonalized to obtain a new set of Bogoliubov transformation coefficients $W^{(1)}$ which are used to compute a new density matrix $\mathcal{R}^{(1)}$. The process is reaped until convergence, that is $\mathcal{R}^{(n+1)} - \mathcal{R}^{(n)}$ is smaller than some threshold parameter ϵ (typically of the order of 10^{-6}). There is no guarantee that this iterative process is converging to a solution and often situations where the iterative process jumps back and forth between two densities are common. To improve upon this situation, some degree of "annealing" is introduced in such a way that the n density matrix is mixed back with the density of step $n-1$ and a weight λ

$$\mathcal{R}^{(n)} = (1-\lambda)\mathcal{R}^{(n)} + \lambda\mathcal{R}^{(n-1)}$$

Choosing conveniently the weight λ convergence is achieved in most of the cases. There are however more attractive methods to solve the HFB equation that are based on the origin of the equation, namely the determination of the absolute minimum of the HFB energy as a functional of the Z parameters. Those are standard minimization methods, like the gradient method, that use the derivative of the energy with respect to the variational parameters to determine a direction in the multidimensional space to proceed towards the minimum. To be more precise, the gradient method uses

$$\mathbb{Z} = -i\eta[\mathbb{R}, \mathbb{H}]^*$$

to determine the wave function of the next iteration. If the step size η is small enough we have $\delta E = -\frac{\eta}{2}\sum_{\mu\nu} |[\mathbb{R}, \mathbb{H}]|^2_{\mu\nu}$ which is a negative quantity (that is we are in the right direction in our search for the minimum energy). The determination of η is kind of an art as it has to be small enough as to always gain energy but large enough to reduce the iteration count to a manageable number. In this respect, second order gradient methods that include information of the curvature (second derivative) are advantageous as they allow to guess a reasonable value of η apart from modifying the gradient's direction to achieve the feat of minimizing an exactly quadratic form in just a single iteration.

Let us finally mention that the HFB equation has to be solved with the constraint on particle number that the mean value of the particle number operator equals proton and neutron numbers, that is $\langle N \rangle = N$, $\langle Z \rangle = Z$. As the origin of the HFB equation is variational we only have to replace the energy functional by

$$E' = E - \lambda_Z \langle Z \rangle - \lambda_N \langle N \rangle$$

where the Lagrange multipliers λ_Z and λ_N allow for an unconstrained minimization and have to be adjusted to impose the desired constraint. The introduction of constraints requires the replacement of the hamiltonian matrix

$$\mathcal{H} \implies \mathcal{H} - \lambda_N \mathcal{N} - \lambda_Z \mathcal{Z}$$

and some strategy to determine the Lagrange multipliers (or chemical potentials are usually denoted). In the gradient method the chemical potentials are determined by requiring that the chosen direction has to be orthogonal to the gradient of the constraints, that is

$$[\mathbb{R}, \mathbb{H} - \lambda_Z \mathbb{Z} - \lambda_N \mathbb{N}] : \mathbb{Z} = [\mathbb{R}, \mathbb{H} - \lambda_Z \mathbb{Z} - \lambda_N \mathbb{N}] : \mathbb{N} = 0$$

that is a linear system of two equations for the two chemical potentials. The constraints are not only used to fix the number of particles on the average but also to study the response of the systems to external perturbations modifying, for instance, the nucleus' multipole moments as in the studies of fission. By introducing a constraint on the mean value of the angular momentum operator J_x

$$\langle J_x \rangle = \sqrt{I(I+1) - \langle J_z^2 \rangle}$$

the HFB cranking model is defined. It allows to study high spin physics (mostly rotational bands) where the lowest energy state with angular momentum I is determined. The so called self consistent cranking (SCC) is routinely used to study the high spin physics of deformed nuclei. The main characteristic differentiating the cranking model from others is the explicit breaking of time reversal invariance imposed by the J_x constraint. It brings some technical difficulties that will not be discussed here.

It has to be stressed that the formalism just developed is independent of the kind of quasiparticle density considered and therefore is valid (with some small adjustments) to describe the HFB equation for odd-A systems (blocked HFB) and also the HFB equation for finite temperature systems.

VI. SOME EXAMPLES

In the following I will present some examples of application of the HFB theory to describe some physical cases. I have chosen examples where I am an author of the corresponding publication not because I consider the calculation superior to others but just for the easy access to the figures presented. Therefore, all the examples presented will correspond to calculations with the finite range Gogny force.

The first calculation corresponds to the potential energy felt by an isotope of Nobelium in its way to fission through a quadrupole deformation of its ground state [4]. In this case the HFB equation for ^{254}No is solved by constraining on the mean value of the axially symmetric quadrupole moment $\langle Q_{20} \rangle$. The energy thus obtained $E(Q_{20})$ is plotted in the figure as a function of Q_{20} (in barn=100 fm^2). Several curves are represented depending on the inclusion of beyond mean field effects (ZPE) or the consideration of reflection symmetric solutions ($Q_{30} = 0$). Along with the curves, the real matter density isosurface is plotted

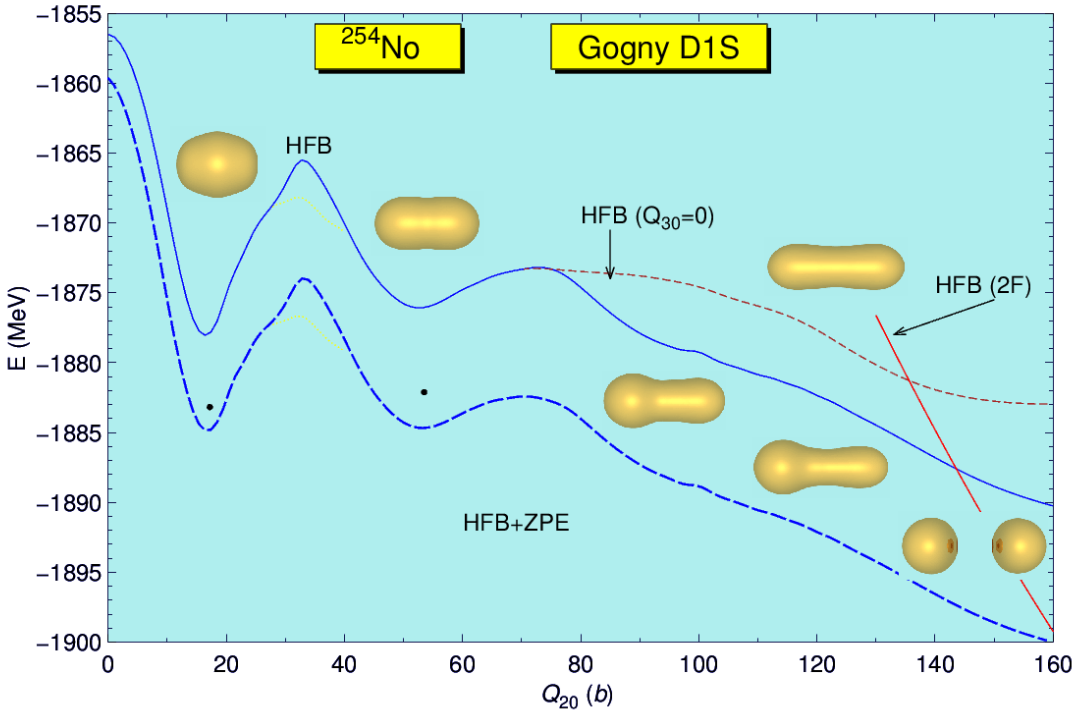

Figure 3: Fission path to fission for the nucleus ^{254}No

for relevant quadrupole moments. An evolution to a two fragment solution is observed. The lowest energy one breaks reflection symmetry and therefore leads to a fission split with different mass fragments in good agreement with the experimental results.

In the second example another constrained calculation constrained on the quadrupole moment of the nucleus around the spherical configuration is performed [5]. The aim of this study is the understanding of some low lying 0^+ states in neutron deficient Pb isotopes that are thought to be associated to different nuclear shapes (oblate deformation, spherical and prolate one). This constitutes probably the most outstanding example of shape coexistence in the atomic nucleus. In the plot the HFB energy is plotted as a function of the quadrupole deformation q or the β_2 deformation parameter (upper x axis). Three minima are observed in all the cases considered that correspond to prolate, spherical and oblate minima. The isosurface of the matter density is plotted again along with the energy. The nuclei studied are some neutron deficient lead isotopes.

We now turn to an example of high spin physics described by the self consistent cranking model [3]. The nucleus under consideration is ^{164}Er that is known as a paradigmatic example

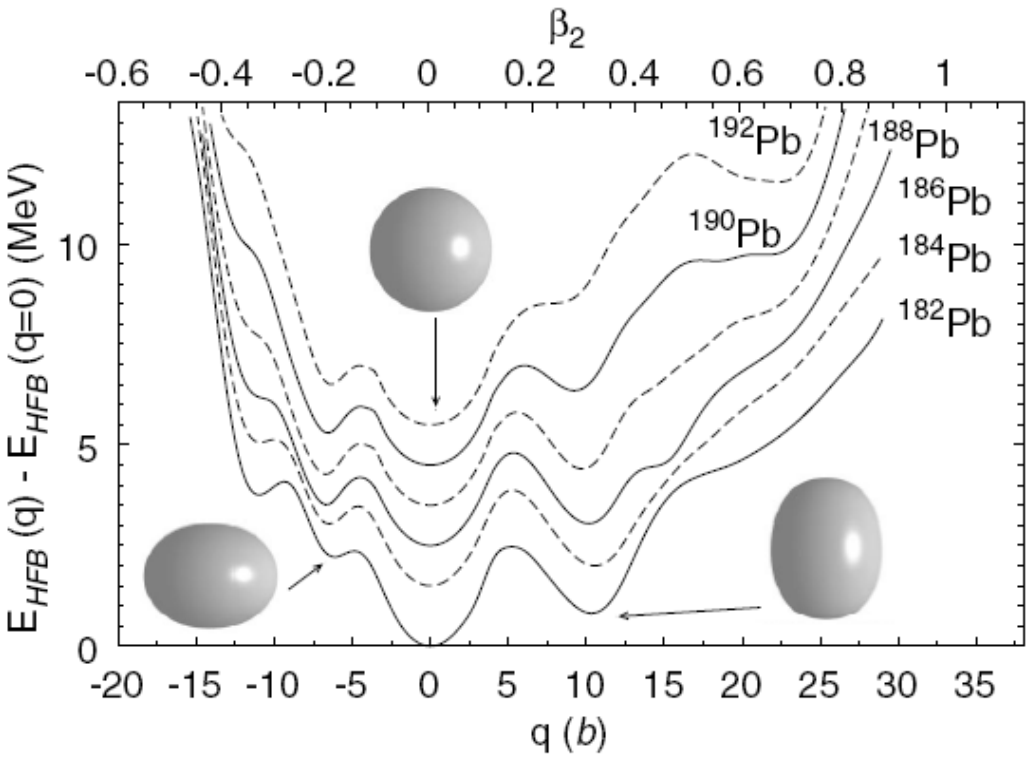

Figure 4: Shape coexistence in neutron poor Pb isotopes, as describer with a constrained calculation with the Gogny D1S interaction.

of rotational band showing the backbending phenomenon. In the upper panel of the plot the gamma ray energy obtained from the HFB energy ($\Delta E = E(I) - E(I-2)$)) is plotted as a function of the angular momentum of the state of the rotational band I. An steady increase with I is observed up to $I = 14\hbar$ where a small dip is observed and the steady increase is recovered at angular momentum $I = 18\hbar$. This is the celebrated backbending phenomenon present in a wealth of rotational bands all over the nuclear chart. As we can observe, the theoretical results reproduce nicely this delicate effect and allow to understand its origin. The original lowest energy rotational band (that increases quadratically with I) crosses at $I = 14\hbar$another excited rotational band with lower curvature. The curvature of the energy of the rotational band as a function of I is proportional to the inverse of the "moment of inertia" of the rotational band. The static moment of inertia $\mathcal{J}^{(1)}$ is plotted as a function of I in the lower panel of the figure as a function of the angular velocity ω which is proportional to ΔE. The backbending gives rise to the characteristic "S" shape of the moment of inertia. Before the backbending the moment of inertia corresponds to the ground

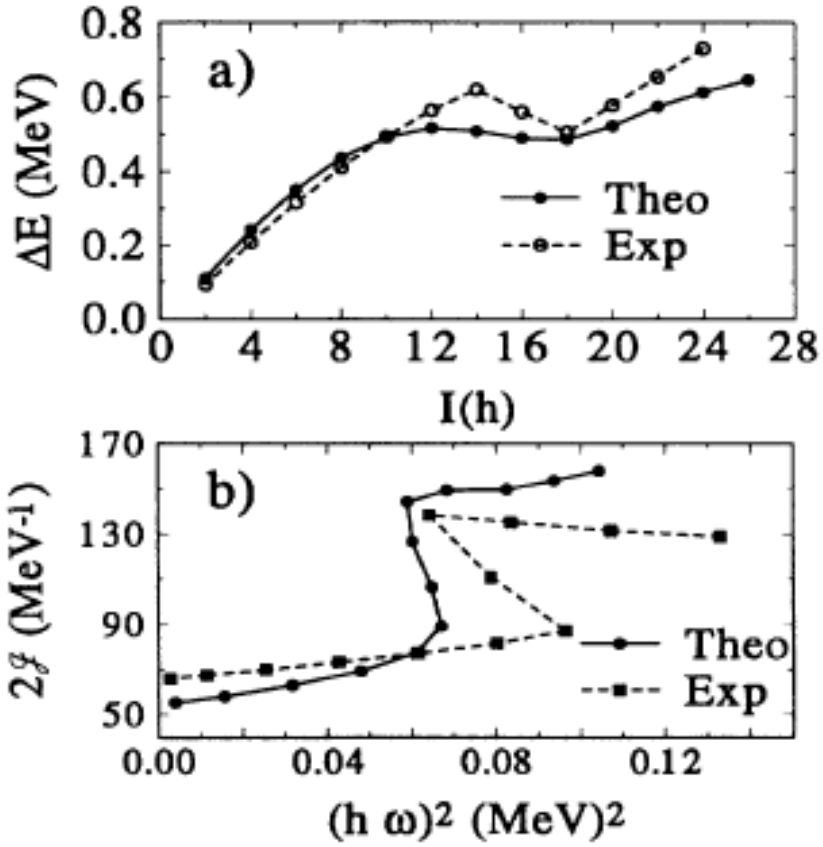

Figure 5: Backbending phenomenom in the nucleus ^{164}Er as described by self consistent calculations with the cranking model and the Gogny force D1S

state band whereas after the backbending the moment of inertia is larger and corresponds to the excited band that, in crossing the ground state band, is at the origin of backbending.

To finish this flashy overview of HFB results let me mention the calculation [11] of the lowest lying energy spectrum of several odd-A isotopes of Radium that show the phenomenon of reflection symmetry breaking (octupole deformation). Octupole deformation leads to a pear like matter distribution similar to the one sketched in the figure 6.

The structure of the odd-A radium isotopes is computed with a variant of the blocked HFB equation that preserves time reversal invariance by replacing the pure HFB by an statistical version where a given orbital and its time reversed partner are both present in the statistical admixture with the same probability (the celebrated Equal Filling Approximation, EFA). Each of the states presented are obtained by blocking different HFB quasi-particles

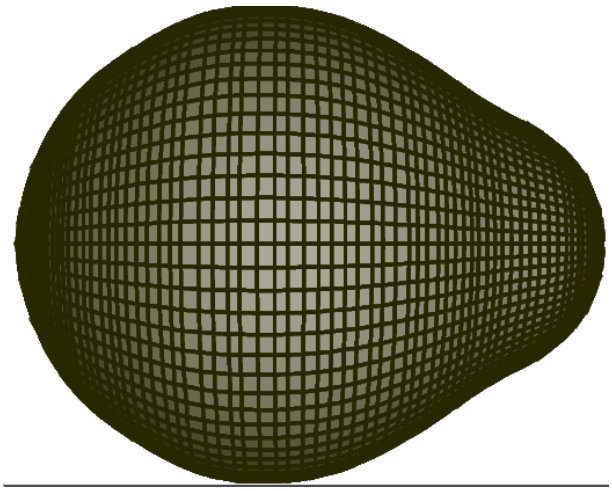

Figure 6: Realistic shape of an octupole deformed nucleus in its ground state (^{224}Ra). The characteristic reflection asymmetry is clearly observed.

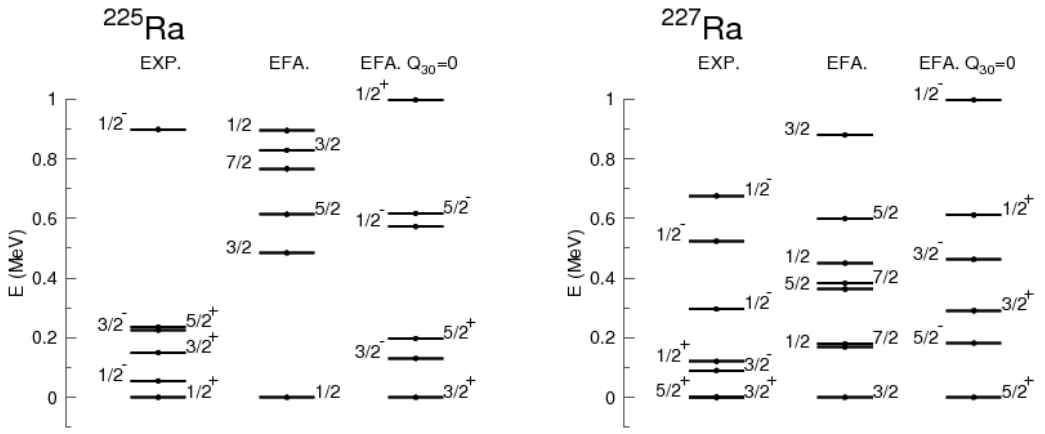

Figure 7: Excitation spectrum of two Ra isotopes as computed with the EFA and the Gogny D1S interaction. The results of two sets of calculations, one preserving reflection symmetry and the other not, are compared to the experimental spectrum.

with different values of the K quantum number (the projection of angular momentum along the z axis).

Let me finish this overview of the mean field method by mentioning the present status of the method and its applications to describe physical properties of the nucleus. At present the HFB theory is used with effective interactions/functionals to describe the binding energies of nuclei all over the nuclear chart with an accuracy that achieve a mean square

radius average as low as 0.6 MeV for the HFB-21 model or 0.7 MeV for Gogny D1M. Also the relativistic mean field models achieve a very good performance in this respect. This impressive reproduction of binding energies comes together with a reasonable description of radii. However, it turns out that the required precision for astrophysical applications is still higher. Also the divergence of predictions for nuclei away from the stability line, in the realm of neutron rich regions, call for additional improvements of the interactions/models and also for the consideration of beyond mean field effects that would be the subject of the next lectures. With those effective interactions it is also possible to reproduce many other properties of nuclei ranging from deformation parameters to moments of inertia or fission half lives. The computed codes required to perform the calculations are available to the community and the calculations can be performed within the day in most of the cases in a personal computed. There is no reason why those HFB based models should not be used by the experimentalists to interpret their results.

There is a vast number of nuclei that have not been extensively studied with mean field methods: they are the odd-A and odd-odd nuclei. The reason is that the HFB theory has to be replaced by the "blocked HFB". The blocked HFB break time reversal invariance and has many more relevant solutions depending upon the quasiparticle to be blocked. Those technical difficulties are in the process of being softened and in the near future the application of the HFB theory to those odd-A and odd-odd nuclei would be as easy as it is now for even-even systems. Another field that would benefit from the developments in the implementation of the HFB theory is the field of K isomers and multiquasiparticle excitations. Those physical systems can be described using the same "blocking" techniques as in the odd-A case but considering the blocking of more than one particle at a time. The study of those systems will allow to extend our understanding of nuclear structure from the traditional field of collective excitations to the still to be explored one of isomers and multiquasiparticle excitations.

Last but not least, the physics of highly excited configurations could potentially benefit from the developments of the HFB theory at finite temperature and efforts to study fission at finite temperature are, for instance, of interest at present.

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