# Symmetry breaking and symmetry restoration in mean-field based approaches

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# ABSTRACT

Mean field approaches are widely used for studying the structure properties of nuclei. Indeed, the mean field approximation is a powerful theoretical tool capable of describing all kinds of nuclei, in particular the heavy, open-shell ones for which the configuration space becomes too large for ab-initio or shell-model approaches. Mean field approaches have the advantage of describing nuclei in terms of simple wave functions, e.g. a single Slater determinant, and they are able to take into account important kinds of correlations between nucleons. However, this is usually at the price of breaking several of the symmetries of the underlying many-body Hamiltonian. For instance, the long range particle-hole correlations responsible for stable deformations and the particle-particle correlations that induce superfluidity can be treated by the Hartree-Fock-Bogoliubov theory, an approach that violates both angular momentum and particle number conservations, respectively.

In principle, symmetries have to be restored. This is especially necessary in two cases. First, if we are interested in nuclear spectroscopy i.e., the energies of the discrete levels and the transition probabilities between them. Indeed, meaningful results require that the wave functions carry good quantum numbers, in particular good angular momentum. Second, in the case of weak symmetry breaking where important correlations take place which cannot be adequately described by mean-field wave functions. In these cases, symmetries can be restored by using projection techniques or, more generally the Generator Coordinate Method, a class of beyond-the-mean-field approaches involving coherent superpositions of continuous sets of mean-field wave functions.

In this report, Section I is devoted to the mean field approach. The Hartree-Fock equations are first sketched and symmetry violating solutions that are of major interest in nuclear physics are then discussed. In Section II, the restoration of symmetry is presented, and recent applications to nuclear spectroscopy are discussed in Section III. Finally, recent and future developments are sketched in Section IV.

# I. THE MEAN-FIELD APPROXIMATION

# 1. The Hartree-Fock equations

In the mean field approximation, we suppose that each particle interacts with an average field generated by all the other particles. The basic ingredient of a mean field approach is the effective Hamiltonian which governs the dynamics of the individual nucleons. It contains a kinetic term and a

two-body effective interaction (in the form of e.g., the Skyrme (see [Chabanat97] and [Chabanat98] for the Sly parameterizations) or the Gogny force [Dechargé80], [Berger91]):

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^2}{2M} + \frac{1}{2} \sum_{i \neq j=1}^{A} v_{ij}^{eff}.$$
 (1)

In the Hartree-Fock theory, the mean-field potential is determined from a variational principle:

$$\delta \langle \Phi | H | \Phi \rangle = 0, \qquad (2)$$

.

with  $\Phi$  a Slater determinant, i.e. an anti-symmetrized products of the A orbitals of the nucleons, as trial wave function:

$$\Phi = \det \left| \varphi_1(x_1) \varphi_2(x_2) \varphi_3(x_3) ... \varphi_A(x_A) \right|.$$
(3)

The variational principle leads to the Hartree-Fock equations – a set of coupled Schrodinger equations:

$$\left[\frac{-\hbar^2}{2M}\nabla^2 + U_{HF}(\varphi_{\alpha})\right]\varphi_i(x_i) = \varepsilon_i\varphi_i(x_i), \qquad (4)$$

with  $U_{HF}$  the Hartree-Fock mean field and  $\varepsilon_i$  the energy of the nucleon level i. The solutions are single particle or hole states, i.e. individual nucleon states completely empty or fully occupied.

In open-shell nuclei, the last occupied level, the Fermi level, is usually not entirely occupied. To define the ground state in a unique manner, it is necessary to introduce the effect of the residual interaction by going beyond the HF approximation. In these nuclei, the part of the residual interaction that comes first into play is the pairing interaction. A natural way to introduce the pairing interaction and to continue working in the framework of the mean-field approximation is to use the Hartree-Fock-Bogoliubov (HFB) formalism. Details about the Hartree-Fock-Bogoliubov approach can be found in [Ring80].

Let us note that HF(B) equations -see Eq. (4)- are non-linear. In the past, for the sake of simplicity, and for reduced computing time, symmetries were often imposed, such as sphericity, axial symmetry, ... Nowadays due to high computer power, new HFB codes have been built, where all these symmetries can be broken [Dobaczewski05].

#### 2. Symmetry violating mean-field solutions

As already stated, the mean-field approximation allows us to describe the system in terms of simple wave functions (Slater determinant). However, the mean field usually breaks several of the symmetries of the nuclear Hamiltonian. Indeed, when the variational principle is performed, the solutions that minimize the total energy may not respect these symmetries. The first example of such a symmetrybreaking is translational invariance which is always broken because the HF orbitals are solutions of a localized mean-field.

This can be illustrated by the schematic example of two interacting particles with masses  $m_1$  and  $m_2$ . In such a case, the Hamiltonian writes - for a harmonic 2-body interaction - :

$$H = -\frac{\hbar^2}{2m_1} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m_2} \frac{\partial^2}{\partial x_2^2} + \frac{1}{2} k(x_1 - x_2)^2.$$
(5)

Let us consider a solution as:

 $\Phi(x_1, x_2) = \varphi_1(x_1)\varphi_2(x_2)$  (6)

The variational principle

$$S \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0, \tag{7}$$

leads to, if  $\varphi_1(x_1)$  and  $\varphi_2(x_2)$  eigenstates of the parity,

$$\begin{cases} \left(-\frac{\hbar^{2}}{2m_{1}}\frac{\partial^{2}}{\partial x_{1}^{2}}+\frac{1}{2}kx_{1}^{2}\right) \varphi_{1}^{i}(x_{1}) = h_{1}\varphi_{1}^{i}(x_{1}) = \varepsilon_{1}\varphi_{1}^{i}(x_{1}) \\ \left(-\frac{\hbar^{2}}{2m_{2}}\frac{\partial^{2}}{\partial x_{2}^{2}}+\frac{1}{2}kx_{2}^{2}\right) \varphi_{2}^{i}(x_{2}) = h_{2}\varphi_{2}^{i}(x_{2}) = \varepsilon_{2}\varphi_{2}^{i}(x_{2}). \end{cases}$$
(8)

The solutions of these equations are, for the ground state,

$$\varphi_{i}^{0}(\mathbf{x}_{i}) = (\sqrt{\pi}b_{i})^{-1/2}\exp(-\frac{1}{2}(\frac{\mathbf{x}_{i}}{b_{i}})^{2})$$
 (9)

with  $b_i = \frac{\hbar}{\sqrt{m_i k}}$ .

We clearly see that such wave functions of Eq.(9) are non translational invariant.

In a similar way, HF wave-functions of a nuclear system break the translational invariance, since the spatial one body density of the system is localized in space.

The second example of symmetry breaking is related to the rotational invariance, which is broken in all deformed nuclei-. As illustrated in FIG 1, where the mean deformation of the HFB ground state is plotted for all even-even nuclei from proton drip-line to neutron drip-line [Hilaire07], only a few nuclei are predicted to be spherical, those associated to neutron magic numbers, and to a lesser extent the ones associated to proton magic numbers. In all the other nuclei, the minimum of energy if found for a non-zero quadrupole deformation. In such a case we have:

$$H_{exact}, J = 0$$
 but  $H_{HF}, J \neq 0$ 

with J the angular momentum operator,  $H_{exact}$  the exact Hamiltonian of the many-body problem, and  $H_{HF}$  the Hartree-Fock Hamiltonian of Eq. (4).



# FIG 1: Predictions for the deformation of the ground states of all even-even nuclei from proton drip line to neutron drip line, obtained from HFB calculations with the Gogny force [Hilaire07].

Let us mention that symmetry breaking is a means to introduce correlations that would not exist if the mean-field respected all symmetries of the Hamiltonian. For instance, in the latter case of FIG 1, the symmetry-violating mean-field approach takes into account the long range particle-hole correlations responsible for stable deformations. Indeed, with strong correlations a symmetry-violating minimum develops. In analogy to solid state physics, the system undergoes a phase transition to a symmetry-violating state such as a deformed state or, in the case of pairing correlations, a superfluid phase. Such a feature is illustrated in FIG 2 where the energy of the system is plotted as function of a variable q (an order parameter) in two typical cases of breaking and non –breaking symmetry<sup>1</sup>.



# FIG 2: Schematic representation of the energy of a symmetry conserving and a symmetry non conserving solution.

<sup>&</sup>lt;sup>1</sup>. However, we must pay attention to the fact that the concept of a sharp phase transition is only valid for infinite systems. In finite nuclei the transition is smeared.

In the self-consistent HF(B) formalism the energy curves of FIG 2 can be generated by means of constraints, i.e. of external fields represented by operators appropriate to the nature of the order parameter q, for instance in the case of deformation by the isoscalar quadrupole deformation  $\hat{Q}_{20}$ 

The intrinsic deformed states of the system are then taken as the solutions of the constrained HF(B) variational principle:

$$\delta \left\langle \Phi_{q} \left| H - \lambda \hat{Q}_{20} \right| \Phi_{q} \right\rangle = 0, \qquad (10)$$

where the Lagrange parameter  $\boldsymbol{\lambda}$  is deduced from the condition

$$\left\langle \Phi_{q} \left| \hat{Q}_{20} \right| \Phi_{q} \right\rangle = \mathbf{q}.$$
 (11)

To continue the comparison with phase transition in solid state physics, we consider the order parameter q, whose magnitude (and phase) monitores the breaking of the symmetry. With an appropriate definition of q, symmetry-breaking solutions are found for  $q\neq 0$  values and symmetry-conserving solutions for q=0 (as illustrated in FIG 2). Let us mention that in case of a continuous symmetry breaking, the energy is independent of the phase of the order parameter, and we get the famous Mexican hat picture (see FIG 3).



# FIG 3: Energy of the solution as a function of the magnitude and phase of the order parameter q also called Mexican Hat (figure taken from [Duguet10])

The mean-field symmetry-breaking solutions in fact provide only a preliminary description of physical system and symmetries must eventually be restored. The HFB state can be seen as a wave packet over the order parameter q and restoring symmetries can be done by using an enriched trial wave function that carries good quantum numbers, and contains more correlations than mean-field ones.

Another very important consequence of symmetry restoration is that it leads to the breaking of the degeneracy of the ground state, and to the appearance of low-lying collective modes [(see Section III.1 for examples in nuclear physics), that are experimentally observed.

#### II. SYMMETRY RESTORATION

#### **1.** Separation of variables

For the translational invariance, the effect of the symmetry breaking on the energy can approximately be taken into account quite easily. However, let us mention that it is a very difficult task to define a wave function, which is translational invariant. Such a task is nonetheless mandatory as long as we want to correct other observables than energy.

To correct the energy of the system, the kinetic energy of the center-of-mass motion has to be subtracted from the Routhian to be minimized in order to ensure that the center of mass is kept at rest. Indeed, let us consider a Hamiltonian defined as a function of the coordinates  $r_i$ :

$$H = -\frac{\hbar^2}{2m} \sum_{i} \left(\frac{\partial}{\partial r_i}\right)^2 + V.$$
 (12)

We first perform a change of the coordinates and we introduce R the center of mass coordinate and  $x_i$  the coordinates in the center of mass frame:

$$\begin{cases} x_i = r_i - R \\ R = \frac{1}{A} \sum_i r_i \\ P = \frac{\hbar}{i} \frac{\partial}{\partial x_i} \\ P = \frac{\hbar}{i} \frac{\partial}{\partial R} \end{cases}$$

We define:

The Hamiltonian of Eq. (12) writes:

$$H = \frac{1}{2Am}P^{2} + \sum_{i} \frac{p_{i}^{2}}{2m} + V - \frac{1}{2Am} (\sum_{i} p_{i})^{2}$$

Such a Hamiltonian can be separated into a collective part and an intrinsic one. The intrinsic Hamiltonian writes :

$$H_{\rm int} = \sum_{i} \frac{p_i^2}{2m} + V - \frac{1}{2Am} (\sum_{i} p_i)^2.$$
(13)

Let us mention that this procedure, in principle, is not so simple [Ring80]. Indeed, the intrinsic Hamiltonian (7) does not depend on the 3A coordinates of the A particles, but only on 3A-1 variables  $x_i$  (the A<sup>th</sup> coordinate being the center of mass R). None of these  $x_i$  variables can then be identified with particle position coordinates and it is not possible to describe easily the intrinsic motion within the independent particle picture. However, such a problem can be solved by using the method of redundant coordinates (such an approach introduces spurious solutions among the eigenfunctions, which have to be eliminated by usual techniques [Ring80].)

To take into account the influence of the breaking of the translational symmetry on the energy, Eq. (13) shows that we have to subtract from the usual HF(B) Hamiltonian the term

$$\frac{1}{2Am} (\sum_{i} p_i)^2$$

This defines an intrinsic Hamiltonian corrected from the spurious energy associated with translationalsymmetry breaking. The above correction that is introduced in the HF(B) equations is called the center of mass correction. It contains two terms, namely a one-body and a two body corrections:

$$\frac{1}{2Am} (\sum_{i} p_{i})^{2} = \frac{1}{2Am} (\sum_{i} p_{i}^{2} + \sum_{i \neq j} p_{i} p_{j})$$

Of course, the two-body term is more complicated and costly to calculate than the one-body term. For that reason, it was often omitted in the past in mean-field calculations. However for the sake of consistency and also because the two-body correction is important in heavy nuclei (the one-body correction decreases with A and is larger in light nuclei whereas the two-body one increases because of the double sum), both center of mass corrections have to be introduced.

For symmetries other than translation, the transformation of variables into an intrinsic frame and the construction of an intrinsic Hamiltonian are difficult, because a complete separation between collective and intrinsic degrees of freedom cannot be achieved. A more general way to treat symmetry violations then is to use the projection methods based on the Generator Coordinate Method (the Random Phase Approximation technique is not covered in this lecture. See E. Khan lecture)

#### 2. Projection methods

Let us consider a symmetry-violating wave function  $|\phi\rangle$ , for instance the HFB wave function of a deformed nucleus, and let us apply the elements R( $\Omega$ ) of the rotation group onto  $|\phi\rangle$ 

$$|\phi(\Omega)\rangle = R(\Omega)|\phi\rangle.$$

It can be shown [Ring80b] that there exists a function  $f(\Omega)$  such that the state

$$\left|\Psi\right\rangle = \int\!\!d\Omega\;f(\Omega) \Big|\phi(\Omega)\big\rangle$$

has the correct symmetry, and whose form can be deduced from symmetry group considerations. However  $f(\Omega)$  contains unknown parameters and the full function can be obtained through a minimization principle. Such an approach then is similar to the Generator Coordinate Method [Hill53] [Griffin57].

For example, let us consider the restoration of the particle number. We start with a HFB wave function  $|\phi\rangle$  which is not an eigenstate of the particle number operator but possesses only the average particle number  $\langle \hat{A} \rangle = A$ 

The decomposition of the HFB wave function into components of good particle numbers can be represented schematically as in FIG 4.



FIG 4: Schematic decomposition of a HFB wave function into components of good particle numbers.

Mathematically this decomposition can be written

$$|\Psi\rangle = \sum_{n} f_{n} \hat{P}^{2n} |\phi\rangle,$$

where

$$P^{A} = \frac{1}{2\pi} \int_{0}^{2\pi} e^{i\varphi(\hat{N}-A)} d\varphi$$

is the projection operator over the exact particle number A. If we are interested in the component of

 $|\Psi\rangle$  with the proper A, then we should take  $f_n=0$  for  $2n\neq A$ , and  $f_n=1$  for 2n=A.

In practice, wave functions with both good angular momentum and good particle numbers are obtained by using several projection operators:

$$\left| JMq \right\rangle = \sum_{q} F^*{}_{Jk} \hat{P}^J_{MK} \hat{P}_{N_0} \hat{P}_{Z_0} \left| \phi_q \right\rangle,$$

where the set of wave function  $|\phi_q\rangle$  is generated by mean-field calculations with constraints on several collective coordinate q (see Eq. (10)).  $P_{MK}^{J}$ ,  $P_{N0}$ ,  $P_{Z0}$  are, respectively, projectors onto angular momentum *J* with projection *M* along the laboratory *z*-axis, neutron number *N* and proton number *Z*. The operator  $P_{MK}^{J}$  extracts from an intrinsic wave function the component with a projection *K* along the intrinsic *z*-axis [Sabbey07].

$$\hat{P}^{J}_{MK} = \frac{2J+1}{16\pi^2} \int d\alpha \int d\beta \sin\beta \int d\gamma D^{*J}_{MK}(\alpha,\beta,\gamma) \hat{R}(\alpha,\beta,\gamma),$$

with  $D_{MK}^{*J}(\alpha, \beta, \gamma)$  the Wigner rotation matrix,  $\hat{R}(\alpha, \beta, \gamma)$  the rotation operator, and  $\alpha, \beta, \gamma$  the usual Euler angles.

#### 2. Configuration mixing calculations

The angular momentum projection introduces part of the quadrupole correlations, since it mixes states with different orientations, i.e. the different components of the quadrupole tensor. In order to fully take into account quadrupole correlations, configuration mixing calculations on the collective variable q can be performed for each angular momentum. The mixed projected many-body state writes:

$$\left| JMk \right\rangle = \sum_{q} f_{Jk}(q) \left| JMq \right\rangle$$

and the weight functions  $f_{Jk}$  are found by requiring that the expectation value of the energy, is stationary with respect to an arbitrary variation  $df_{Jk}$ . The Hill-Wheeler equation writes:

$$\sum_{q} (H_{J}(q,q') - E_{k}I_{J}(q,q'))f_{Jk}(q') = 0$$

with

$$\begin{split} H_{J}(q,q') &= \left\langle JMq \left| \hat{H} \right| JMq' \right\rangle, \\ I_{J}(q,q') &= \left\langle JMq \right| JMq' \right\rangle \end{split}$$

Solutions of the Hill-Wheeler equation, for each value of the angular momentum J, are: the ground state, and excited states orthogonal to the ground state.

### 3. Collective Hamiltonian

An alternative (approximate) method to the full Generator Coordinate Method, is to use the Gaussian overlap approximation to construct a collective Hamiltonian. One starts with the constrained Hartree-Fock-Bogoliubov (CHFB) theory of the potential energy surface, and constructs a collective Hamiltonian from the potential energy surface and the information about the kinetic energy operator (mass parameters...).

In the case of the 5-dimensional quadrupole collective variables, CHFB calculations with constraints on the Bohr deformation variables  $\beta$  and  $\gamma$  are performed, and the collective states are obtained from the diagonalization of a 5-dimensional collective Hamiltonian [Kumar67] which is formally similar to the Bohr Hamiltonian. It has six kinetic terms, associated with the three rotational moments of inertia and three mass parameters associated with the coupled dynamics of axial and triaxial deformations. The collective Hamiltonian writes:

$$\hat{H}_{coll} = \frac{1}{2} \sum_{k=1}^{3} \frac{\hat{I}_{k}^{2}}{J_{k}} - \frac{1}{2} \sum_{m,n=0 \text{ and } 2} D^{-1/2} \frac{\partial}{\partial a_{m}} D^{1/2} (B_{mn})^{-1} \frac{\partial}{\partial a_{n}} + V(a_{0},a_{2}) - \Delta V(a_{0},a_{2}),$$

with  $a_0 = \beta \cos \gamma$  and  $a_2 = \beta \sin \gamma$ . Here,  $\beta$ , and  $\gamma$  are the Bohr deformations, V is the HFB potential energy,  $\Delta V$  the so-called zero-point energy correction, I<sub>k</sub> the angular momentum operator and J<sub>k</sub> the associated inertia about the k axis, B<sub>mn</sub> the mass parameters, and D a metric defined as [Libert99]:

$$D = (B_{00}B_{22} - B^2_{02})\prod_k J_k.$$

This approach allows us to obtain rotational states coupled to axial and triaxial quadrupole vibrations.

# **III. EXAMPLES FROM NUCLEAR PHYSICS**

#### 1. General features

In nuclear physics, the many-body Hamiltonian is invariant under translation, rotation, parity, and z-signature, and conserves nucleon numbers.

Table I displays the general features associated to the translational, rotational and particle number symmetries in HF calculations.

| Name          | Commutation            | In which   | Due to ?    | Order       | Quantum                    |
|---------------|------------------------|------------|-------------|-------------|----------------------------|
|               | rules                  | Nuclei ?   |             | parameter   | numbers of the             |
|               |                        |            |             |             | excitations                |
| Translational |                        | All        | Localized   | d           | $I^{\pi}=1^{-}$            |
| symmetry      | $[H_{HF}, P] \neq 0$   |            | mean-field  |             | T=0                        |
| Rotational    |                        | Deformed   | Deformation | Quadrupole  | $I^{\pi}=0^+,2^+,4^+\dots$ |
| symmetry      | $[H_{HF}, J^2] \neq 0$ |            |             | deformation | T=0                        |
| Particle      |                        | Superfluid | Pairing     | gap         | $I^{\pi} = 0^+$            |
| number        | $[H_{HFB}, N] \neq 0$  |            |             |             | $T=T_0, T_0=2$             |

TABLE 1: Order parameter and quantum numbers of the excitations associated to symmetry breaking and restoration. I is the spin,  $\pi$  the parity and T the isospin. For the definition of d see [Schuck86].

In Table I, in the last column are given the quantum numbers of the excitations associated with the spontaneous breaking of each kind of symmetry. For instance, in an even-even nucleus, the excitations associated to the breaking of the rotational invariance, constitutes the T=0 rotational band  $0^+$ ,  $2^+$ ,  $4^+$ ... Let us mention, that in the reference [Schuck86] such excitations are called "Goldstone modes". They are obtained by beyond mean-field calculations restoring symmetries, and they reflect the spontaneous breaking of the symmetry at the mean field level.

FIG 5 illustrates the relation between the observed low-lying levels and the predicted deformation. Results in the Samarium chain shows that the vibration mode becomes softer with respect to the deformation. We observe a regular lowering of the first  $2^+$  state from <sup>148</sup>Sm to <sup>154</sup>Sm, together with an increase of the deformation predicted by mean-field calculations. Let us note that the spectrum of <sup>148</sup>Sm is a typical vibrational spectrum with equally-spaced levels, whereas the spectrum of <sup>154</sup>Sm is a typical rotational one, with a spacing between the levels following the rule of I(I+1)/2J, with I the spin and J the moment of inertia.



<sup>Sm</sup> FIG 5: Breaking of the spherical symmetry and low-energy spectroscopy in even-even Sm isotopes. (Courtesy of D. Goutte)

# 2. Ground state correlations

State of the art calculations using projection methods can be found in the literature. Among the most accomplished, we discuss here the results obtained by M. Bender, et al., about *Global study of quadrupole correlation effects* [Bender06], where the authors analyze how large are the correlation energies associated with broken symmetries, and symmetry restoration. Indeed, in heavy systems, the binding energy is around 1000 MeV, and the different parameterizations of the effective forces give a rms around 1 MeV. How large are the energy gained by symmetry breaking and symmetry restoration with respect to this value of 1 MeV?

In this systematic study the static deformation energy is predicted to be between 0 and 12 MeV, depending on the nucleus. The energy gain from particle number and angular momentum projections amounts for 1.4 to 4.2 MeV and the energy gain from quadrupole vibrations for around 1 MeV. Finally, the total dynamical correlation energy is between 1.5 and 5 MeV. Such a value is much larger than the accuracy of the present approaches for nuclear masses determination [Moller08] [Goriely09], and cannot then be neglected.

#### 3 Low energy spectrum

We discuss now the results obtained for low-energy collective states, and in particular the first  $2^+$  observed in even-even nuclei. In different works the properties of the lowest  $2^+$  excited state have been analyzed over the whole periodic table. There are 557 even-even nuclei with known  $2^+$  excitation energies as of compilation by Raman *et al.* in 2001 [Raman01]. Their excitation energies span more than 2 orders of magnitude, presenting a very substantial challenge to any global theory of nuclear structure.

Theoretical excitation energies obtained using the 5-dimensional collective Hamiltonian approach (5DCH) and the Gogny force D1S are compared with experimental data on FIG 6 [Bertsch07]. The lowest energies are for the actinides; it is in this region of heavy deformed nuclei that the theoretical energies are the most accurate. On the contrary, at high excitation energies (1 MeV and higher), the theory displays only a qualitative predictive power. A large discrepancy also appears for a few neutron deficient isotopes of mercury and lead, where the low-lying weakly deformed oblate and well-deformed prolate structures are not well reproduced.

A systematic study of  $2^+$  state energies has also been performed by Sabbey *et al.* [Sabbey07]. In this latter reference, a zero range Skyrme force has been used, and configuration mixing calculations have been performed using the full GCM formalism, where the configurations generated by the GCM have been projected on angular momentum and particle numbers. This theory does very well on the quadrupole properties of deformed nuclei. However, the calculated collective energies are systematically higher than in the 5DCH case. At this time it is not clear what the origin of the difference is (dependence on the functionals and/or theoretical approximations?)



# FIG 7: Comparison between theoretical predictions and experimental energies of the first 2<sup>+</sup> state in even-even nuclei [Bertsch07].

Other yrast and yrare excited states have been calculated with the same approaches from drip-line to drip-line [Delaroche10]. Recently, results from the 5DCH approach have been made available on two repository sites [Database10] for nuclei with Z=10 – 110 and N< 200, for ground states properties such as charge radii, 2n separation energy, correlations energy and quadrupole moment, yrast band up to the 6<sup>+</sup> and yrare states  $0^+_2$ ,  $2^+_2$  and  $2^+_3$ .

# **VI Future developments**

Many theoretical developments related to symmetry breaking and symmetry restoration in mean-field based approaches have been undertaken these last few years. Among them, we mention here some very promising:

- First full triaxial angular momentum projections are under developments. First results have been obtained in <sup>24</sup>Mg [Bender08] [Rodriguez10]. In a few years, a systematic study of full 3 D projections in the entire nuclear chart will be undertaken.

- Full variation after projection calculations have been undertaken by different groups. Indeed, in the aforementioned GCM calculations, projections are performed after variation, i.e., solutions are not obtained from a proper variational principle. Pioneering works have already been published along this line [Rodriguez02] [Rodriguez05] and [Stoitsov07]].

- A derivation of a formal framework for GCM-type calculations to avoid spurious contributions to the energy density functional has been developed [Duguet09] [Lacroix09] and [Bender09]. Such developments should now be implemented in the codes.

For the future, particle number and angular momentum projection applied to odd nuclei would be extremely valuable. That would allow us to calculate states of good spin that could be directly compared to experimental data.

Finally, most of the projection calculations have been performed up to now only in the framework of nuclear structure. Similar calculations should be performed in the domain of nuclear reactions. Indeed, an accurate description of reaction mechanisms should involve nuclear wave-functions having good particle numbers, and good angular momentum. A first attempt of using a projection technique to calculate transfer probabilities in  ${}^{16}O+{}^{208}Pb$  reaction below the fusion barrier has been made recently [Simenel10] and the results are very encouraging. What about the importance of the projection on particle number when describing the fission process?

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