Microscopic approach to collective motion

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An overview of a microscopic framework based on the Hartree-Fock description of the mean field is presented which, starting from an effective interaction allows a description of collective motions. A study of the isotope shifts in the Pb region illustrates the importance of the effective interactions and points to their limitations. Such forces should be improved in order to achieve a better description of nuclei properties especially with the coming availability of exotic beam facilities. The coupling of collective quadrupole and octupole degrees of freedom in ^{194}Pb is analyzed within the Generator Coordinate Method, which represents a step beyond the simple mean-field approximation. As a last example, we present a study of nuclear rotations. First we discuss results on superdeformed rotating bands in ^{192}Hg, ^{194}Hg and ^{194}Pb obtained without including a treatment of pairing correlations. Preliminary calculations are also presented with these correlations included as well as an approximate projection on nucleon number.

1. THEORETICAL OUTLINE

Two types of basic ingredients can be found in most mean field calculations; first a two-body nucleon-nucleon effective interaction, such as a Skyrme-type one, complemented by a pairing interaction. The many body wave function representing the nucleus is approximated by a Slater determinant or a BCS state. Then a minimization of its energy yields

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the Hartree-Fock (HF) or mean field equations. These equations are non linear as the mean potential depends upon the solution through different densities (mass, kinetic energy...) in addition to the explicit density dependent terms which appear due to the density dependence of the effective interaction. The numerical solution is performed via an iterative procedure from an initial guess of the solution. In practical calculations, the BCS equations for the pairing interaction are solved at each HF iteration so that pairing correlations are included self-consistently into the mean field and not only in first order perturbation theory as when pairing is treated as a residual interaction. Since the HF equations result from a variational principle, the solution is an energy extremum, the absolute minimum being obtained when the initial conditions are properly chosen.

After the choice of the interaction comes the second key ingredient to describe collective motions in mean field calculations, namely a set of constraining operators which are included to explore these collective degrees of freedom. The minimization of this modified energy functional yields the constrained Hartree-Fock (CHF) equations [1–3]. As before, their solution gives a Slater determinant representing the many body wave function of the nucleus, subject to the chosen constraints. The choice of the constraining operator (or operators) depends upon the physics. Degrees of freedom associated to the shape of the nucleus are studied mostly by means of quadrupole constraints [1]. As an example, we will present below an analysis [4] of the quadrupole-octupole coupling in ^{194}Pb in which both octupole and quadrupole operators have been added to the HF mean field. Similarly, the fission path of heavier nuclei can be studied with a quadrupole constraint together with a hexadecapole one. In every cases, the resulting shape of the nucleus is *optimized* with respect to all other unconstrained operators, e.g. of other multipolarities, due to the variational nature of the CHF equations.

To study rotating nuclei, one generally adds a constraint on the projection of the angular momentum onto the appropriate axis [5]. To generate rotational bands in superdeformed (SD) nuclei, a constraint on the quadrupole deformation is also introduced to construct the SD secondary minima on which one wants to build a rotational band. In the Hg region, where such secondary minima do exist at zero angular momentum, the quadrupole constraint can be released when the nucleus is cranked up. Whereas in other regions of the mass table, no such minimum exists and one must keep the quadrupole constraint until the angular momentum is high enough to stabilize the deformation.

In all these cases, nuclei are described by intrinsic states which usually break several symmetries. In particular they are no longer eigenstates of the angular momentum operators, nor of the particle number operators when pairing correlations are included. Only the mean value of these operators is accounted for through the constraining fields.

We have considered two methods which allow to get a better description of the nuclear properties beyond the mean field approximation. The first one is the Generator Coordinate Method (GCM) which provides collective wave functions associated to a given mode [6]. Let us make three comments, i) in all the cases we have studied until now, this method reduces to a diagonalization of the residual interaction in the configuration space built on a finite set of constrained intrinsic HF states, with the additional technical difficulty that these states are not orthogonal. ii) these HF states which generate the GCM basis are bound by the collective potential: we never considered situations involving scattering states. The collective wave functions which we calculate represent bound

states within the collective well. iii) finally, as the generating states are built from the same (Skyrme) interaction which is used in the GCM calculation, the dimension of the GCM basis remains rather small. Typically 30 to 40 CHF states at most are usually required to describe quadrupole deformations from oblate to prolate SD shapes and even hyperdeformed (HD) ones for axially symmetric configurations. If one were to use another set of generating states, this number would be much larger. Somehow this number is minimal when the generating states incorporate most of the mean field effects of the two body interaction used in the GCM.

The second method realizes the restoration of broken symmetries through projection. This can be done in two ways, the simplest method consists in projecting the HF solution onto good quantum numbers. Along this line, particle number projection has been done in some cases [7]. Angular momentum projection has also been performed in an approximate manner by an appropriate use of the specific symmetries of the triaxial GCM in the Sr region [8]. A second and more accurate way involves a projection before variation. Since it is rather difficult to implement, we have resorted the Lipkin-Nogami (LN) prescription [9, 10] which emulates an approximate projection up to the second order in $\hat{N} - < \hat{N} >$ onto the particle number operator $\hat{N}$ before variation.

In what follows, we illustrate the main points which have been listed above. First we present a study [11] of the isotope shifts of Pb nuclei to emphasize the importance of the choice of the effective interaction and discuss their range of validity. Then we present an analysis of the quadrupole-octupole modes in ^{194}Pb together with a GCM calculation of the corresponding collective wave functions [4]. Finally a study of identical bands in the Hg-Pb region is given without pairing correlations [12]. Preliminary calculations with these correlations included are also presented and the effect of restoring symmetry breaking is discussed in the case of an approximate projection onto good particle number via the LN prescription. The choice of these topic aims at covering the different aspects of mean field calculations, namely: definition of an effective force, choice of the collective variables (or equivalently constraining operators), exploration of collective correlations beyond the mean-field, and finally partial restoration of symmetry breaking.

2. ISOTOPE SHIFTS OF THE PB NUCLEI

The isotope shifts of atomic levels provide a very good testing ground for nuclear forces. They are experimentally measured with a high accuracy. From their values, the variation of root-mean-square charge radii can be obtained with little ambiguity. The Pb isotope sequence is particularly interesting as the ^{208}Pb doubly-magic nucleus is one of the anchor points in the parametrization of effective interactions for mean field calculations.

The behavior of the r.m.s. radii presents too features. One is a kink at the ^{208}Pb shell closure when they are drawn as a function of the mass number. The other one is an odd-even staggering. These features are not specific to the Pb isotopic chain and are observed in other region of the mass table [13].

2.1. Mean field calculations

We have calculated the proton radii with three different Skyrme forces. First we used SIII [14] which is one of the most successful Skyrme force for spectroscopic properties. However it has a rather large incompressibility modulus ($K_\infty = 355$ MeV) and predicts

too large fission barriers. Then we used SkM* [15] and SGII [16] which are derived from the SkM force [17]. The latter is intended to give correct energies for isoscalar $E0$ and isovector $E1$ giant resonances whereas SkM* improves upon surfaces tension to allow studies of fissioning nuclei. Both SkM* and SGII have a smaller value of K_∞ than SIII.

Figure 1. Proton (circle) and neutron (squares) mean-square radii of Pb isotopes for different Skyrme forces. The experimental points are connected by a dotted line.

We define changes in mean square radii with respect to ^{208}Pb as $\Delta r^2(A) \equiv r_2(A) - r_2(208)$, where $r_2(A)$ is the mean square radius of the isotope of mass A whose wave function is calculated within HFBCS. Fig. 1 shows calculated and experimental proton $\Delta r^2(A)$ as a function of the mass number. To all these quantities we have subtracted the change in mean square radii of a liquid drop, $\Delta r^2_{\rm LD}(A) \equiv r^2_{\rm LD}(A) - r^2_{\rm LD}(208)$, with $r^2_{\rm LD} = \frac{3}{5} r_0^2 A^{2/3}$ and $r_0 = 1.2$ fm. This subtraction emphasizes deviations from any smooth trend.

If the agreement with experiment is excellent for SkM* and SGII for neutron deficient isotopes, all calculations fail to reproduce the abrupt change in slope at $A = 208$. As the slope is almost linear both sides of ^{208}Pb, we characterize this change in slope by its *kink* defined from ^{194}Pb, ^{208}Pb, and ^{214}Pb as $k \equiv \frac{1}{6}\Delta r^2(214) - \frac{1}{14}\Delta r^2(194)$. The values of k are given in table 1 with those of Δr^2, both for protons and neutrons. The size of the kink is larger for neutrons, which is natural as the proton radius can only change through the p-n attractive force when one varies the neutron number for a given charge. A stronger p-n

Table 1
Differences of proton and neutron radii (fm^2) from those of ^{208}Pb calculated with three types of Skyrme forces.

force	$\Delta r_{\rm p}^2$		$k_{\rm p}$	$\Delta r_{\rm n}^2$		$k_{\rm n}$
	(^{194}Pb)	(^{214}Pb)		(^{194}Pb)	(^{214}Pb)	
SkM*	−0.7573	0.3545	0.0050	−1.5931	0.8530	0.0284
SIII	−0.8680	0.4481	0.0127	−1.4939	0.8335	0.0322
SGII	−0.7448	0.4576	0.0231	−1.4589	0.8843	0.0432
exp	−0.6830	0.6099	0.0529			

force would result in a larger kink, however, as the neutron kink is smaller than the proton experimental one, it is unlikely that the sole modification of the symmetry properties of the force will resolve the discrepancy. Let us also note that the magnitude of k is not directly related to the incompressibility modulus. The SkM* and SGII forces give very different values of k, although they have the same value of K_∞. The kink obtained for SIII lies in between whereas its K_∞ is much larger. Finally, Hartree Fock Bogoboliubov (HFB) calculations have also been done [18] with the D1S interaction [19,20]. They produce a kink of 0.12 fm^2 which is as small as that of SIII.

It is important in a study of the isotope shifts based on an effective force to verify the quality of that force for the calculated binding energies. With ^{208}Pb as a reference point, fig. 2 shows the predicted binding energy difference, $\Delta E(A) \equiv E(A) - E(208)$, to which we have subtracted the equivalent experimental quantity. The analysis of this figure shows that $\Delta E(A)$ strongly deviates from zero. This implies that none of these three forces can be considered to have correct symmetry energy properties.

Nevertheless, from the present calculation, it appears to us that SIII is the best choice among these three forces. Indeed it gives results comparable in quality as one moves away either side of ^{208}Pb. Had we chosen ^{194}Pb as a reference point to calculate Δr^2 and ΔE, none of the three forces would have predicted the ^{208}Pb binding energy correctly, however SIII alone would have given a remarkable agreement for ^{214}Pb, with $\Delta E < 100$ keV and $\Delta r^2 < 0.023$ fm^2.

2.2. Corrections

To improve upon these mean field calculations, we have calculated different corrections. First of all the experimental isotope shifts measure a difference in charge radii whereas HF calculations give a proton density. We have then folded the proton density with the charge distribution of the proton, taking into account effects coming from the neutron charge distribution and the spin density [21]. These effects are small and roughly proportional to the mass number. They modify slightly the charge radii of the three nuclei we use to calculate the kink which does not change in a significant manner, less than 1%

The experimental isotope shifts depend mostly upon the mean square charge radii, however higher moments of the charge density also enter in their determination. The ratio of the contribution of these higher moments to that of the mean square radius is estimated assuming a uniform charge distribution [22,23]. We extracted from our calculations the expectation values of r^4 and found that even though the expectation values of both r^2

Figure 2. Error of calculated masses of Pb isotopes with SGII (dashed line), SkM* (solid line), and SIII (squares). Differences are plotted with respect to ^{208}Pb.

and r^4 are overestimated in the sharp density model, their ratio agrees rather well with our numbers. It is thus very unlikely that any refinement of the experimental analysis will provide an explanation for the kink.

The above corrections remain within the scope of the predictions from a mean field calculation. We have also investigated possible corrections coming from the admixture of collective modes into the HFBCS ground states, extending our calculations beyond the mean field approach. This is done by utilizing the GCM where the generating variable is chosen according to the mode we want to study. In all these GCM calculations, we have used the SkM* interaction. Quadrupole modes were first studied in this way. The resulting modification is the isotope shifts is very small, at most 1% in ^{194}Pb, even smaller in ^{214}Pb. A GCM analysis of the isoscalar breathing mode lead to similar results.

None of the above contributions presents dramatic changes across the doubly-magic ^{208}Pb nucleus. Experimentally, the level scheme shows evidence for a modification of the octupole properties when crossing the magic shell closure. For masses smaller than 208, the lowest 3^- state is similar to that of ^{208}Pb although its collectivity decreases as one removes pairs of neutrons. For neutron rich isotopes, additional 3^- states can be constructed from the excitation of one neutron from the now populated g9/2 shell to the j15/2. On this basis, we have studied possible contribution to the kink from coupling to octupole modes. However, in that case too, the complete GCM calculation did not significantly modify our mean field results.

In view of the smallness of these corrections, we did not think that a more complete two- or even three-dimensional GCM calculation, mixing the three moments together,

Table 2
Neutron and proton mean square radii (in fm^2) with density dependent pairing.

	ρ_c	V_0^n	Δr_p^2		k_p	Δr_n^2		k_n
	[fm^{-3}]	[MeV fm^3]	(^{194}Pb)	(^{214}Pb)		(^{194}Pb)	(^{214}Pb)	
a)	∞	-230	-0.8948	0.3097	-0.0123	-1.7440	0.7930	0.0076
b)	—	g_n=12.5	-0.7573	0.3545	0.0050	-1.5931	0.8530	0.0284
c)	0.1603	-750	-0.6662	0.3753	0.0150	-1.5137	0.8668	0.0364
d)	0.1382	-1150	-0.5165	0.4454	0.0373	-1.3571	0.9453	0.0606
e)	0.13	-1450	-0.4464	0.4761	0.0475	-1.2825	0.9817	0.0720
exp			-0.6830	0.6099	0.0529			

would change our conclusion.

2.3. Density-dependent pairing forces

Instead of the constant G pairing interaction, we use below a more realistic zero-range δ-pairing force [24,25] for the BCS calculation, together with the SkM* nuclear force. We choose to quench this pairing interaction inside the nucleus, as is usually the case of Landau-Migdal particle-hole effective forces [26]. With this choice, the nucleus tends to expand when the pairing correlation is switched on because the interaction is stronger at lower densities, e.g. in the vicinity of the surface. To achieve this quenching, we have introduced density dependence in the pairing interaction as follows:

$$V^\tau(\vec{r}_1,\sigma_1;\vec{r}_2,\sigma_2) = V_0^\tau \frac{1-\vec{\sigma}_1\cdot\vec{\sigma}_2}{4}\delta(\vec{r}_1-\vec{r}_2) f(\frac{\vec{r}_1+\vec{r}_2}{2}). \quad (1)$$

As the density dependence function $f(\vec{r})$, we choose, for the sake of simplicity, linear dependence on the nucleon density parameterized by a critical density ρ_c,

$$f(\vec{r}) = 1 - \frac{\rho(\vec{r})}{\rho_c}. \quad (2)$$

Such a density-dependent parametrization have already been proposed and used in into different physical situations such as the analysis of pairing in the actinide region [27] or a more recent study of pair correlations near the neutron drip line [28]. In these studies, the f function depends upon the density through a fractional power.

One can schematically show how this new pairing force will affect the radius. Assuming a constant density ρ_0 within a sharp surface, the average size of the two-body pairing matrix element is estimated to be, $\bar{v} = (V_0/N)\ \rho\ (1-\rho_0/\rho_c)$, which is maximum at $\rho_0 = \rho_c/2$. In the case of a pure δ-force ($\rho_c = \infty$), pairing compresses the nucleus as compared to the HF solution. If $\rho_c = \rho_0$, pairing is turned off inside the nucleus, it acts as a surface interaction [29] and the nucleus expands.

Table 2 gives the parameters of the neutron pairing force used in the calculation, no proton pairing is considered. The set (a) correspond to a pure δ-force, it tends to compress the nucleus, (b) is our previous constant G pairing calculation for comparison. The sets (c), (d) and (e) correspond to different choices of ρ_c. In case (c), ρ_c is the saturation density of SkM*, while in case (d), it is the density of a liquid drop of radius $1.2A^{1/3}$ fm. When calculated with SkM*, the average interior density of the Pb isotopes is about

0.158 fm^{-3}, which is between (c) and (d). An even smaller value of ρ_c, (e), has been used to show the sensitivity of the kink to this parameter. In all cases, the strength V_0 was adjusted to reproduce the experimental pairing gaps.

If the value of the kink can be fitted to experiment, while adjusting ρ_c, the overall trend of the isotope shift still does not agree with the data. The increase of the kink is obtained by raising both branches of the theoretical curves on fig. 1 until they match to the correct angle, the overall slope however remains the same and thus incorrect. Indeed this is related to the symmetry-energy property of SkM* which has remained almost unchanged: the total binding energies do not vary significantly (less than 0.8 MeV) for ^{194}Pb and ^{214}Pb from case (a) to (e).

2.4. The effective interaction revisited

In the above section, we have shown that the symmetry properties of most used Skyrme forces cannot reproduce the overall behavior of the isotope shifts. This statement holds for the D1S force as well [18]. For SkM*, we have also shown that an adjustment of the pairing interaction can resolve part of the discrepancy. Therefore a more correct procedure should involve first an improvement of the symmetry property of the force, then a tuning of the pairing force, if need be.

In the usual fitting procedures [14,24], the Skyrme parameters are fitted to a limited set of quantities. Among them is the saturation property of infinite nuclear matter and the incompressibility modulus. One also includes ground state properties of a small set of closed shell nuclei together with the surface tension and the symmetry energy. However, these last quantities are known only in the vicinity of the β stability line. Calculations are then carried on for other nuclei throughout the mass region to predict their spectroscopic properties until some experimental evidence shows that new features have to be incorporated in the parametrization of the force.

From this point of view, the symmetry energy property of the force is a local property: if a nucleus is correctly calculated, neighboring ones will be calculated with a similar accuracy. A study of an isotopic chain is exploring the global aspect of the N-Z degree of freedom, this feature has not been taken into account in the adjustment of the force.

To improve on the global symmetry energy, we decided to fit a new set of Skyrme parameters not only to symmetric nuclear matter, but also to the extreme case of dense neutron matter. For that purpose we took the UV14 plus UVII equation of state [30] (eos) and the saturation property of symmetric matter as input to the fit. We have verified that the resulting Skyrme eos does reproduce the normal density neutron matter eos [31]. The next step in the adjustment is to reproduce the binding energies of a limited set of spherical nuclei ranging from ^{16}O to ^{208}Pb within the constraints given by the fit of symmetric and neutron infinite nuclear matter.

For the resulting set of parameters [32], the upper left part of fig. 3 shows the energy difference between the UV14 plus UVII and the Skyrme eos for neutron matter. The other inserts correspond to different Skyrme forces. As one can see, none of the present parametrization reproduces correctly the neutron matter eos of ref. [30], only our new set of parameters does it. As these forces have a similar symmetry energy coefficient, this illustrates that it is only a local measure of the symmetry properties of the force. The success of our fit shows that it is possible to improve them without necessarily modifying

the analytical structure of the Skyrme force or adding new terms into it.

Our fit remains very preliminary, as it should be confronted to more nuclear spectroscopic properties and eventually improved. Finally, isotope shifts are to be calculated again to test the need of a density dependence of the pairing interaction.

Figure 3. Energy differences between various Skyrme and the UV14+UVII equation of state for neutron matter as a function of the neutron density.

3. QUADRUPOLE-OCTUPOLE COUPLING

In the previous microscopic analysis of quadrupole and octupole modes, only one degree of freedom was taken into account in the GCM calculations. In an other work investigating the properties of ^{222}Ra [33], we solved the CHF equations constraining both on the quadrupole and on the octupole operators. No GCM calculation was made, only parity projection was realized. In a later work [34], we studied the octupole softness of the SD

state of ^{194}Pb. For that nucleus, we performed GCM calculations utilizing the octupole as generating variable for different but fixed quadrupole deformation. The octupole constraint was imposed either on Q_{30}, Q_{32} or a combination of these two operators.

3.1. CHF calculations

We are presently pursuing the latter analysis doing two-dimensional GCM calculations for ^{194}Pb, using the SkM* force. We use the conventional G pairing interaction in the BCS formalism. To constrain on the octupole mode, we choose the operator $q_{30} = \langle r^3 Y_{30} \rangle$. The other octupole modes which have not been included in the preesent analysis are of two kinds. First, the q_{32} has been proven to be weakly coupled to the q_{30} mode at small quadrupole deformation and negligible otherwise [34]. The odd components, q_{31} and q_{33}, have also been recently studied and found to generate states which lie at a higher excitation energy than those associated to q_{33} [35].

We have considered quadrupole moments from -40 to 100 barn. This range extends well beyond the SD minimum and covers the HD region. This is illustrated on fig. 4 which shows the CHF energy as a function of the quadrupole moment. In addition to the usual ground state and SD minima, there exists a shallow third minimum around 80 b which is candidate to accomodate a HD state. To decide whether such a state actually exists requires a dynamical calculation.

For each value of quadrupole moment (q_2), we have included states with increasing octupole deformation up to an excitation energy such that the GCM space used in the calculation of the next section was large enough to ensure a good accuracy on the collective spectrum and wave functions. A maximum value of $q_{30} = 7000$ fm^3 was necessary to achieve this calculation. Fig. 4 summarizes for each value of q_{30} the range of q_2 values which has been taken into account and shows the excitation energy domain spanned by our set of CHF basis states.

The main feature which appears on fig. 4 is the softness of the SD minimum with octupole deformation. At $q_{30} = 0$, the SD minimum is 4.67 MeV higher than the absolute one. At $q_{30} = 2000$ fm^3 it is only 1.75 MeV higher, whereas at $q_{30} = 3000$ fm^3, the situation is reversed and the second minimum is now lower than the first one by 0.9 MeV. This feature was already present in the limited calculation of ref [34]. A remarkable result of the present analysis is the bending of the SD valley toward larger quadrupole deformation. When q_{30} increases from 0 to 7000 fm^3, the SD quadrupole moment increases smoothly and continuously from 46 up to 58 barn. In contrast the valley extending in the q_{30} direction from the ground state minimum is much steeper and eventually disappears around 5000 fm^3. The third HD minimum located at 82 barns corresponds to an ellipsoidal shape with a 2.1 to 1 axis ratio. At $q_{30} = 0$, the depth of this well is only 0.8 MeV. When q_{30} is increased, the quadrupole deformation of this third minimum increases but only slightly as it smoothly disappears. At $q_{30} = 5000$ fm^3, only a plateau is observed.

In the case of octupole deformation, HFBCS states with opposite octupole moments may be used to construct eigenstates of the parity operator, realizing thus parity projection, as was in ref. [33,34].

3.2. GCM calculations

Once the CHF states have been constructed, we solved first the simpler GCM equations with the quadrupole moment as a single generating variable ($q_{30} = 0$). In that case the

Figure 4. HFBCS deformation energy curves as a function of q_2 (in barn) for values of the octupole moment ranging from 0 to 7000 fm^3.

lowest GCM state is 1.4 MeV below the absolute minimum of the HFBCS calculation, which is a measure of the quadrupole correlations in the ground state of ^{194}Pb. In all the calculations we present now, we have chosen the energy of this state as the origin of the energy scale. Then we solve the GCM equations with both q_2 and q_{30} as generating variables. As this method has been adequately described in details [6], we will only present here the particular aspect resulting from its generalization to the study of the octupole mode together with the quadrupole one.

The GCM states $\mid \Psi_k\rangle$ result from the diagonalization of the hamiltonian in the nonorthogonal basis of HF+BCS states $\mid \Phi(q_2^i, q_{30}^j)\rangle$ corresponding to different quadrupole and octupole moments, q_2^i and q_{30}^j,

$$\mid \Psi_k\rangle = \sum_{i,j} f_{ij} \mid \Phi(q_2^i, q_{30}^j)\rangle \quad . \tag{3}$$

To solve the Hill Wheeler equations, we have to calculate the norm matrix and the matrix elements of the hamiltonian between all the CHF states $\mid \Phi(q_2^i, q_{30}^j)\rangle$. As in ref [6], the mean particle number of the GCM states is corrected by means of the Lagrange

Figure 5. GCM spectrum of Pb194. The solid line gives the HFBCS energy curve as a function of the quadrupole moment. Even states are marked by a vertical tick-mark, odd ones by a black dot.

Figure 6. Enlargement of the previous figure. States are number with increasing excitation energy. When connected by a dotted line, they correspond to a sequence of states generated by octupole phonon excitations.

multiplier method. Since the parity is preserved by the hamiltonian, the space of GCM solutions is divided into positive and negative parity subspaces which do not interact. Positive and negative parity collective wave functions and spectra were obtained after a careful analysis of the numerical stability of the results related to the truncation of the eigenvalues of the norm matrix on one hand, and of the completeness of the $q_2 - q_{30}$ space on the other hand.

Fig 5 shows the full GCM spectrum. Even parity states are shown with a vertical tickmark at the mean value of their quadrupole moment, odd states with black dots. Due to the octupole correlations, the ground state energy gains an additional 1.4 MeV binding so that it lies 2.8 MeV below the absolute HFBCS minimum. As compared with the GCM calculation without the octupole mode included, all the low lying even states are shifted downward by the same 1.4 MeV energy and have roughly the same mean quadrupole moment. At higher excitation energy, new even states are found. They are be associated to excitations of octupole phonons, as we show below.

There is no state whose mean value of the quadrupole moment is close to the third minimum although some states have components of their collective wave function at the HD deformation. It therefore appears that the HD well is not deep enough so that no GCM states can qualify unambiguously as a hyperdeformed state.

Fig. 6 shows an enlargement of fig. 5. States are numbered with increasing excitation energies. They are joined in bands according to the structure of their collective wave

Figure 7. Probability density contour plots a function the quadrupole and the octupole moments. First and third rows from the bottom correspond to even states, second and fourth to odd states.

function as illustrated on fig. 7 and 8 which show the probability density of these GCM states in the q_2, q_{30} plane. On fig. 7, one sees that the ground state collective wave function (state 1) is localized around $q_2 = q_{30} = 0$, as would be an s state in a two dimensional space. The band (1,5,12,24) forms a sequence of states corresponding to s p d and f waves in the q_{30} direction. The following band, next column of fig. 7, can be obtained from the previous one by a quadrupole excitation. The third and fourth bands are built on the third and fourth even GCM states (states 3 and 4). The fifth band, built on the eighth state, shows the limits of an interpretation of the GCM states in the first well as being combination of independent quadrupole and octupole elementary excitations. The quadrupole character of this last band is more complicated than a simple additional quadrupole excitation on top of the fourth one. However, the sequence of octupole excitations remains visible.

Fig. 8 represents three bands, the first one (left column) is built from the SD even state (7), it also has the nice pattern of a sequence of s, p, d and f states in the q_{30} direction. These four states are localized in the SD well. Their mean quadrupole moment increases slightly toward the deformation of the second well minimum. The lowest SD even state (7) can be viewed as an s wave state located in the SD well. The mean quadrupole moment

Figure 8. Same as fig. 7 for GCM states at large deformations.

of state (17) corresponds to the maximum of the barrier between the main well and the SD well. The band which is constructed on that state, middle column of fig. 8, has a much more complex structure in q_2. However its structure is preserved as one adds more and more octupole phonon excitation, although components at smaller q_2 are less and less important. The last column of the figure shows a tentative assignment of states built by octupole excitation on the most deformed state (29). These states have significant components in the HD region, around 85 barns. The mean value of the quadrupole moment decreases dramatically as one adds octupole phonons. Furthermore, these states are not at all localized in q_2, the dispersion is so large that they cannot be interpreted as HD states.

We have reconstructed rotational bands on each GCM sates, as we did in ref. [34,36], to explore the influence of octupole softness on the stability of SD bands. The decay out of the band constructed on the first even SD state occurs at the same angular momentum that was obtained already. Electromagnetic $E1$ and $E3$ transitions to odd bands in the first well remain much smaller than the $E2$ transitions to the bands constructed on the even states (1), (2), (3) and (4) so that the decay scheme of the even SD band is not modified.

We have also constructed an odd SD rotational band on the odd state (14). All the

Table 3
Energies, quadrupole moments, dynamical $\mathcal{J}_2$ and rigid body $\mathcal{J}_{\rm rig}$ (MeV^{-1}) moments of inertia and angular frequency $\hbar\omega$ at $20\hbar$ for the five SD bands studied in this work.

Band	E (MeV)	$E_{\rm rot}$ (MeV)	Q_0 (fm^2)	$\mathcal{J}_2$ (MeV^{-1})	$\mathcal{J}_{\rm rig}$ (MeV^{-1})	$\hbar\omega$ (MeV)
^{192}Hg	-1507.734	1.74468	4446.009	115.407	119.319	0.17392
^{194}Pb	-1513.777	1.81887	4644.611	110.681	122.365	0.18151
^{194}Pb*	-1511.611	1.73897	4383.145	116.009	120.133	0.17318
^{194}Hg	-1523.683	1.71442	4393.146	117.925	120.300	0.17056
^{194}Hg*	-1523.350	1.73655	4446.266	116.279	120.709	0.17285

possible $E1$, $E2$ and $E3$ transitions to states in the first well remain small compared to in-band $E2$ transitions. However, $E1$ transitions to states of the even SD band are strong so that this odd band, if it were observed, will depopulate at much higher angular momentum than the even SD band and over a wider range of transitions, typically between $24\hbar$ and $36\hbar$. Its decay will feed the ground SD band.

4. ROTATIONAL SUPERDEFORMED BANDS

The Skyrme-cranking equations have been adequately described in [5]. We have chosen ^{192}Hg as a test case to study SD rotational band with the SkM* parametrization of the Skyrme force.

4.1. Cranked Hartree Fock

First, we have performed cranked HF calculations [12] without including pairing correlations as in an earlier work for ^{24}Mg [5]. As a function of J_z, the neutron et proton routhians we obtained are quite similar to those obtained with cranked Wood-Saxon methods [37], although the assignment of Nilsson quantum numbers to our orbitals is not always unambiguous, as discussed in [38]

Experimentally, one SD band has been observed in ^{192}Hg [39,40], identical bands have been seen in ^{194}Pb [41–43] and ^{194}Hg [37,44]. The γ rays of the only band seen in ^{194}Pb have energies identical to those of ^{192}Hg with a precision better than a couple of keV for $12\hbar \leq J_z \leq 30\hbar$. In ^{194}Hg three bands have been observed. The second excited band or band 3 twins with the same ^{192}Hg band for 15 consecutive transitions.

On the $6_{5/2}$ or the $[514]\frac{9}{2}$ proton orbitals, we have built two ^{194}Pb bands referred to below as ^{194}Pb and ^{194}Pb*. Similarly using either the $[512]\frac{5}{2}$ or the $[624]\frac{9}{2}$ neutron orbitals we have constructed two ^{194}Hg bands (^{194}Hg and ^{194}Hg* respectively). Table 3 summarizes our results at $20\hbar$ for these five bands.

The excitation energy of the ^{194}Pb* band relative to ^{194}Pb band is 2.1MeV, while it is only 0.33MeV for the ^{194}Hg*. Fig. 9 shows the differences of γ-ray energies between the four $A = 194$ bands and ^{192}Hg. The γ transition energies for the ^{194}Pb* and ^{194}Hg* bands differ by one to three keV from those of ^{192}Hg over the experimentally observed range of angular momentum. Our calculation predicts slightly larger differences at higher angular momentum ($J_z \geq 32\hbar$). In contrast, the ^{194}Pb and ^{194}Hg bands do not resemble each other nor the ^{192}Hg band. By discrete differentiation of J_z with respect to $\hbar\omega$, we have calculated the dynamical moment of inertia $\mathcal{J}_2$ of these bands as a function of J_z. For

the five bands the HF value of $\mathcal{J}_2$ grows steadily with J_z. This result differs from those of other studies based on either Woods-Saxon [45] or rotating oscillator [46] potentials in which pairing effects have also been neglected. The values of the HF moments of inertia disagree with the observed ones; they are too large for small J_z's and too small at the largest angular momentum $J_z = 40\hbar$. This indicates that data can only be fully understood when the variation of pairing correlations with rotation is correctly taken into account.

Figure 9. Differences of γ-ray energies between the lowest SD band of ^{192}Hg and the four $A = 194$ SD bands: ^{194}Pb (+), ^{194}Pb* ($\times$), ^{194}Hg ($\triangle$) and ^{194}Pb* ($\diamond$). The horizontal dashed lines indicate the $\pm$2keV accuracy, as a measure of band identity.

Table 3 shows that the variations of the quadrupole moments from one band to the other are not related to the changes in dynamical moments of inertia. The ^{194}Pb band has a larger quadrupole moment and a smaller moment of inertia while the situation is reversed for the ^{194}Hg band. In addition, the HF predicted behavior of $\mathcal{J}_2$ versus J_z is contrary to that of the mass quadrupole moment Q_0 which decreases continuously (although by less than 5%) when the angular momentum grows. Neither the dynamical moment of inertia nor the quadrupole moments obey a simple $A^{5/3}$ rule. As expected the rigid moments of inertia follow the same trend as the quadrupole moments. They are always significantly different from the $\mathcal{J}_2$ values.

As was shown in other works [46,47], our calculations indicate that twinning is related

to the filling of specific single-particle orbitals. However our calculations prove that the occupation of these "twinning" orbitals does not generate a modification of those bulk dynamical properties related to rotation. A full understanding of the microscopic self-consistent origin of this rather delicate balance mechanism will require a deeper analysis of the structure of these orbitals and of their interaction with the mean-field.

4.2. Cranked HFB equations – preliminary results

Pairing correlations are becoming weaker as the angular momentum increases. They may be expected to be small in the rare earth region where SD bands are not observed at low spins, although this conjecture remains to be verified quantitatively. In the Hg region, even though these bands are not observed at zero angular momentum, they extend to much lower spin, presumably below $10\hbar$. For this reason, it is necessary to extend the cranked HF mean field so as to include pairing. Because rotation breaks time-reversal symmetry, the BCS approximation is not valid: it is not possible to assume that pairs are built on only two orbitals of the HF mean-field; one cannot escape the full complexity of the HFB equations.

The implementation of the Bogoliubov transformation in the cranked CHF scheme can be summarized as follows (see ref. [48]):

- Given the self-consistent HF mean-field in coordinate space $h(\rho)$, find the eigenvalues and eigenfunctions of $h(\rho) - \omega J_z$ in both positive and negative signature spaces.
- Calculate the relevant matrix elements of the two-body pairing interaction in the basis which diagonalizes $h(\rho) - \omega J_z$. Construct the gap matrix and solve the HFB equations within the space of positive signature. From the corresponding eigenvalues and the eigenvectors, deduce the HFB matrices U and V and the quasiparticle energies E for both signatures.
- Using the matrices U and V, construct the density matrix and the pairing tensor.
- A diagonalization of the density matrix provides occupation numbers and the eigenfunctions (distinct from the eigenvalues of $h(\rho) - \omega J_z$, as ρ and $h(\rho)$ do not commute). From them, one constructs the density matrix in coordinate space which is then used to build the HF hamiltonian $h(\rho)$ associated with the Skyrme force.

This set of equations is solved self-consistently with a separable pairing force which reduces to the seniority interaction when the angular velocity ω vanishes. Its neutron and proton strengthes have been adjusted to reproduce the static pairing properties of nuclei in the neutron deficient Hg-Pb area of the isotope map.

We have calculated the SD lowest band of ^{192}Hg from $J_z = 0$ to $44\hbar$. Several features appear in the calculation: i) the neutron and proton pairing correlations which are introduced in this HFB calculation disappear at $24\hbar$ and $40\hbar$ respectively. ii) the difference between the total HF and HFB energies is smaller than the sum of neutron and proton pairing energies because there is a loss of binding energy in the mean-field contribution. iii) the ratio of the proton to neutron contributions to angular momentum is always less than Z/N; as J_z grows, it decreases since the superfluidity of neutrons is the first to disappear then it increases smoothly to reflect the fast decrease of proton pairing correlations to finally reach the HF value.

Figure 10. Dynamical moment of inertia in MeV^{-1} as a function of $\hbar\omega$.

Figure 10 compares the experimental dynamical moment of inertia to the calculated one within HFB as a function of $\hbar\omega$. At zero frequency, the HFB moment of inertia, $\mathcal{J}_2 = 80$ MeV^{-1}, is slightly smaller than the experimental extrapolation, in contrast with the HF calculation without pairing of ref. [12], $\mathcal{J}_2 = 110$ MeV^{-1}. Then $\mathcal{J}_2$ increases with $\hbar\omega$ much faster than experiment. The disappearance of the neutron pairing correlations at 24 $\hbar$ is reflected on the HFB $\mathcal{J}_2$ by an abrupt reduction. Similarly, when the proton pairing vanishes at $40\hbar$, the HFB moment of inertia reduces to the HF one. The fast increase of the HFB $\mathcal{J}_2$ between 0 and 24 $\hbar\omega$ indicates that pairing correlations do not decreases fast enough with increasing frequency. The sharp reduction at 24 and 40 $\hbar$ is due to their too early and too sudden disappearance.

Rather than discussing the pairing correlations themselves, it seems natural to look for deficiencies in the mean-field (HFB) treatment of these correlations as the nucleus is a finite system. A well established way to improve the HFB description is provided by the

variation after projection (VAP) method on the correct nucleon number. This method leads to heavier but still tractable calculations. From calculations [49] performed for other nuclei and at smaller deformations, VAP is known to suppress the unphysical sharp HFB phase transition and to maintain pairing correlations to higher angular momentum while softening their decrease.

In view of the present results, we have included in the HFB equations the approximate VAP realized by the LN prescription [9]. The resulting dynamical moment of inertia is shown on fig. 10, it rises continuously from 0 to 30 $\hbar$, angular momentum at which we ended this calculation. As expected, neutron and proton pairing decreases smoothly, but do not vanishes. At $30\hbar$, the proton pairing energy is 50% what it is at $0\hbar$, whereas for neutron it is 40%. As the rise in $\mathcal{J}_2$ is too high as compared with experiment, we have arbitrarily decrease strength of the pairing interaction by 10% and repeated our HFB+LN calculation up to higher $\hbar\omega$, reaching an angular momentum of $46\hbar$. As can be seen from fig. 10, the overall behavior of $\mathcal{J}_2$ agrees rather well with experiment from $\hbar\omega = 0$ to 300 keV, however, it fails to reproduce experiment at higher frequency.

Since the dynamical moment of inertia is defined as $(d\hbar\omega/dJ_z)^{-1}$ one expects $\mathcal{J}_2$ to grow until it reaches a maximum and then to decrease to the HF value. This behavior is very much alike that found in other analyses [50,51] both qualitatively and quantitatively. However it is markedly different from the data [52] which shows a steadily increasing moment of inertia up to the largest observed value of $\hbar\omega$ which is above 400 keV.

5. CONCLUSIONS

In this review, we have focused our attention on our work and showed the the predictive power of mean field calculations complemented by the GCM and projection, starting from an effective force of the Skyrme type. For that purpose, we have selected as an illustration some topics, namely the isotope shifts in ^{194}Pb and the effective force, quadrupole and octupole coupling in ^{194}Pb SD collective states and finally, rotation without and with pairing correlations included. Many more physical situations have been or can be also studied. Let us mention only few of them such as a successful analysis of the odd-even staggering in the Pb isotope shift [11], a study of "banana" modes [35] or a detailed calculation of the electric decay rate of some fission isomers [53].

Along the same path, there are other works which in different ways achieve the same goal. For example, instead of Skyrme forces, the finite range D1S interaction [20] has been extensively used. However the GCM equations are not solved exactly, rather the different groups utilizing D1S make use of the Gaussian Overlap Approximation which yields a collective Bohr Hamiltonian. For instance, SD bands have been analyzed in the Hg region [54]. Still with D1S, the Madrid group has calculated spectroscopic properties of nuclei ranging from the rare earth region [55] to Xenon nuclei [56]. Let us also mention a recent work where they have projected their collective wave function onto good angular momentum to calculate transition probabilities [57]. Finally relativistic mean field approach [58,59] has been applied to calculate nuclear properties. Results obtained so far are quite promising [60].

REFERENCES

1. P. Bonche, H. Flocard, P.H. Heenen, S.J. Krieger and M.S. Weiss, Nucl. Phys. **A443** (1985) 39
2. P. Bonche, S.J. Krieger, Ph. Quentin, M.S. Weiss, J. Meyer, M. Meyer, N. Redon, H. Flocard and P.H. Heenen, Nucl. Phys. **A500** (1989) 308
3. S.J. Krieger, P. Bonche, M.S. Weiss, J. Meyer, H. Flocard and P.H. Heenen, Nucl. Phys. **A542** (1992) 43
4. J. Meyer et al. in preparation
5. P. Bonche, H. Flocard and P.H. Heenen, Nucl. Phys. **A467** (1987) 115
6. P. Bonche, J. Dobaczewski, H. Flocard, P.H. Heenen and J. Meyer, Nucl. Phys. **A510** (1990) 466
7. P.H. Heenen, P. Bonche, J. Dobaczewski and H. Flocard, Nucl. Phys. in press
8. P. Bonche, J. Dobaczewski, H. Flocard and P.H. Heenen, Nucl. Phys. **A530** (1991) 149
9. H.J. Lipkin, Ann. Phys. (New-York) **9** (1960) 272
   Y. Nogami, Phys. Rev. **134** (1964) B313
10. L. Bennour, P.H. Heenen, P. Bonche, J. Dobaczewski and H. Flocard, Phys. Rev. **C40** (1989) 2834
11. N. Tajima, P. Bonche, H. Flocard, P.H. Heenen and M.S. Weiss, Nucl. Phys. **A551** (1993) 434
12. B.Q. Chen, P.H. Heenen, P. Bonche, M.S. Weiss and H. Flocard, Phys. Rev. **C46** (1992) 1582
13. E.W. Otten, Nuclear radii and moments of unstable nuclei, Treatrise in heavy ion science, vol. 8, ed D.A. Bromley (Plenum, New York, 1988) p. 515
14. M. Beiner, H. Flocard, N. Van Giai and Ph. Quentin, Nucl. Phys. **A238** (1975) 29
15. J. Bartel, Ph. Quentin, M. Brack, C. Guet and H.-B. Håkansson, Nucl. Phys. **A386** (1982) 79
16. N. Van Giai and H. Sagawa, Phys. Lett. **B106** (1981) 379
17. H. Krivine, J. Treiner and O. Bohigas, Nucl. Phys. **S336** (1980) 155
18. J.F. Berger, private communication.
19. D. Gogny, in Proc Int. Conf. on Nuclear Physics, eds J. De Boer and H. Mang, (North Holland, Amsterdam, 1973)
20. J. Dechargé, M. Girod and D. Gogny, Phys. Lett. **55B** (1975) 361
    J. Dechargé and D. Gogny, Phys. Rev. **C21** (1980) 1568
21. J. Martorell and D.W.L. Sprung, Z. Phys. **A298** (1980) 153
22. R.C. Thompson, M. Anselment, K. Bekk, S. Göring, A. Hanser, G. Meisel, H. Rebel, G. Schatz, and B.A. Brown, J. of Phys. **G9** (1983) 443
23. U. Dinger, J. Eberz, G. Huber, R. Menges, S. Schröder R. Kirchner, O. Keppler, T. Kühl, D. Marx and G.D. Sprouse, Z. Phys. **A328** (1987) 253
24. F. Tondeur, Nucl. Phys. **A315** (1979) 353
25. S.J. Krieger, P. Bonche, H. Flocard. Ph. Quentin and M.S. Weiss, Nucl. Phys. **A517** (1990) 275
26. J. Speth, E. Werner and W. Wild, Phys. Rep. **C33** (1977) 127
27. R.R. Chasman, Phys. Rev. **C14** (1976) 1935

28. G.F. Bertsch and H. Esbensen, Ann. Phys. **209** (1991) 327
29. I.M. Green and S.A. Moszkowski, Phys. Rev. **139** (1965) B790
30. R.B. Wiringa, V. Fiks and A. Fabrocini, Phys. Rev. **C38** (1998) 1010
31. B. Friedman and V.R. Pandharipande, Nucl. Phys. **A361** (1981) 502
32. E. Chabanat et al. in preparation
33. P. Bonche, P.H. Heenen, H. Flocard and D. Vautherin, Phys. Lett. **175B** (1986) 387
34. P. Bonche, S.J. Krieger, M.S. Weiss, J. Dobaczewski, H. Flocard and P.H. Heenen, Phys. Rev. Lett. **66** (1991) 876
35. J. Skalski, P.H. Heenen, P. Bonche, H. Flocard and J. Meyer, Nucl. Phys. **A551** (1993) 109
36. P. Bonche, J. Dobaczewski, H. Flocard, P.H. Heenen, S.J. Krieger, J. Meyer and M.S. Weiss, Nucl. Phys. **A519** (1990) 509
37. M.A. Riley et al. Nucl. Phys. **A512** (1992) 178
38. M. Meyer et al. Phys. Rev. **C45** (1992) 233
39. D. Ye et al. Phys. Rev. **C41** (1990) R13
40. J.A. Becker et al. Phys. Rev. **C41** (1990) R9
41. M.J. Brinkman et al. Z. Phys. **A336** (1990) 115
42. K. Theine et al. Z. Phys. **A336** (1990) 113
43. H. Hübel et al. Nucl. Phys. **A520** (1990) 125c
44. E.A. Henry et al. Z. Phys. **A335** (1990) 361
45. R.R. Chasman, Phys. Lett. **B219** (1989) 227
46. I. Ragnarsson, Nucl. Phys. **A520** (1990) 67c
47. J. Dudek, Z. Szimanski and T. Werner, to be published
48. H. Flocard, B.Q. Chen, B. Gall, P. Bonche, J. Dobaczewski, P.H. Heenen and M.S. Weiss, Nucl. Phys. **A557** (1993) 559c
49. P. Ring and P. Schuck, The Nuclear Many-Body Problem, Springer Verlag, (1980)
50. R.R. Chasman, Phys. Lett. **B242** (1990) 317
51. E.F. Moore et al., Phys. Rev. Lett. **64** (1990) 3127
52. M.G. Porquet, private communication
53. S.J. Krieger et al., unpublished
54. M. Girod, J.P. Delaroche, J. Libert and I. Deloncle, Phys. Rev. **C45** (1992) R1420
    J. Libert, J.F. Berger, J.P. Delaroche and M. Girod, Nucl. Phys. **A553** (1993) 523c
55. J.L Egido and L.M. Robledo, Phys. Rev. Lett. **70** (1993) 2876
56. V. Martin and L.M. Robledo, Phys. Rev. C, in press
57. J.L Egido, L.M. Robledo and Y. sun, Nucl. Phys. **A560** (1993) 253
58. B.D. Serot and J.D. Walecka, Adv. Nucl. Phys. **16** (1986) 1
59. Y.K. Gambhir, P. Ring and A. Thimet Ann. Phys. (N.Y.) **198** (1990) 132
60. J.P. Maharana, Y.K. Gambhir, J.A. Sheikh and P. Ring, Phys. Rev. **C46** (1992) R1163