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Superdeformed rotational bands in the Mercury region; A Cranked Skyrme-Hartree-Fock-Bogoliubov study

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Abstract

A study of rotational properties of the ground superdeformed bands in ^{190}Hg, ^{192}Hg, ^{194}Hg, and ^{194}Pb is presented. We use the cranked Hartree-Fock-Bogoliubov method with the SkM* parametrization of the Skyrme force in the particle-hole channel and a seniority interaction in the pairing channel. An approximate particle number projection is performed by means of the Lipkin-Nogami prescription. We analyze the proton and neutron quasiparticle routhians in connection with the present information on about thirty presently observed superdeformed bands in nuclei close neighbours of ^{192}Hg.

1 Introduction

With the recent evolution in γ-ray multidetectors, the experimental knowledge of superdeformed (SD) bands in nuclei of the mercury region is rapidly growing. Since the initial discovery of a SD rotational band in ^{191}Hg [1], more than forty bands have been observed for isotopes of Au, Hg, Tl and Pb (see refs. [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12] and the earlier papers cited in the compilation of experimental data [13]). The anchor point of the region appears to be the nucleus ^{192}Hg which corresponds to the SD magic numbers: Z=80 and N=112.

Although superdeformation has been predicted by many models (for a review see ref. [14]), the spectrum of approaches used up to now to study high spin properties of the SD states is still rather limited. The theoretical analyses have been mostly done in terms of the cranked Nilsson-Strutinsky [15] method, either with the modified harmonic oscillator (MHONS), e.g. ref. [16], or with the Wood-Saxon (WSNS), e.g. ref. [17, 18, 19], potentials. The methods relying on a mean field derived from a microscopic nucleon-nucleon force have been applied only in two cases. For ^{192}Hg, ^{194}Hg and ^{194}Pb the cranked Hartree-Fock equations have been solved [20] and in ^{192}Hg the Bohr hamiltonian approach with the collective potential and mass parameters calculated at zero spin has been used [21].

In view of their general good quality at describing zero-spin properties, the latter methods should be more extensively tested at high spins. Such methods are free from geometric assumptions concerning a detailed parametrization of the nuclear surface, and therefore they seem to be more apt at describing polarization phenomena that may appear in the dynamical behaviour of a rotating nucleus.

As compared to the other major region of superdeformation (around A=150) the high spin properties of nuclei in the ^{192}Hg region seem to be different because of the presence of large pairing correlations. In particular, the generally observed increase of the $\mathcal{J}^{(2)}$ moment of inertia is interpreted [22, 23] as resulting both from the alignment of intruder orbitals and from a gradual disappearance of pairing correlations. The relative importance of these two effects requires further microscopic investigations. There exist also uncertainties concerning the predictions of crossing frequencies, the determination of pairing strengths and the evaluation of the relative importance of dynamical pairing

correlations compared to those described by the static pairing formalism which is usually sufficient to account for zero spin properties.

The present work is devoted to a presentation of the cranked Hartree-Fock-Bogoliubov (HFB) method and to a discussion of its ability to address such issues. The next section contains a short description of our theoretical approach. In particular, we present a method of solution of the cranked HFB equations with the Skyrme interaction in the coordinate representation. Pairing correlations are described by a seniority interaction and we briefly describe how we implement an approximate variation after projection by means of the Lipkin-Nogami approach [24, 25, 26] (HFBLN).

As a first application we use the cranked HFB method to study the SD bands in nuclei around ^{192}Hg. Section 3 contains a presentation of our results. First we investigate properties of the ground SD bands in ^{190}Hg, ^{192}Hg, ^{194}Hg and ^{194}Pb. Then, we show that the properties of SD bands observed in other odd and even nuclei in this region are compatible with our spectra of quasiparticle routhians. The last section presents our conclusions.

2 The HFBLN method

2.1 THE TWO-BASIS METHOD

First, we review the cranked HFB method [27] as much as required to introduce our notation. Given the hamiltonian $\hat{H}$ which in a single particle basis $\{a_i^+,\, a_i, (i = 1, \ldots, N)\}$ has the form

$$\begin{aligned} \hat{H} &= \hat{T} + \hat{V} \quad , \\ \hat{T} &= \textstyle\sum_{ij} T_{ij} a_i^+ a_j \quad , \\ \hat{V} &= \tfrac{1}{4} \textstyle\sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_l a_k \quad , \end{aligned} \tag{1}$$

this method determines the quasiparticle vacuum state $|\Psi\rangle$ which minimizes the energy

$$\mathcal{E} = \langle \Psi | \hat{H} | \Psi \rangle \tag{2}$$

subject to the constraints $\langle \Psi | \hat{N} | \Psi \rangle = N_0$ and $\langle \Psi | \hat{J}_x | \Psi \rangle = J_0$. The average value of the particle-number operator $\hat{N}$ is thus constrained to the desired number of nucleons N_0 (separately for neutrons and protons) and that of the cranking operator $\hat{J}_x$ to the desired value of angular momentum[1] J_0. The collective-cranking operator $\hat{J}_x$ is equal to the projection of the angular-momentum vector $\hat{\boldsymbol{J}}$ on the axis perpendicular to the largest-elongation axis.

The determination of $|\Psi\rangle$ amounts to finding the unitary matrix $\mathcal{W}$ which relates the particle creation and annihilation operators $\{a_i^+,\, a_i\}$ to the quasiparticle operators

[1] In general, J_0 is related to the angular momentum J and its projection K on the symmetry axis by $J_0 = \sqrt{J(J+1) - K^2}$. Since we are mostly interested in high spin properties and K=0 bands we take $J_0 \approx J$.

$\{b_i^+, b_i\}$ such that the b's are destruction operators associated with the quasiparticle vacuum $|\Psi\rangle$ ($b_i|\Psi\rangle = 0$, $i = 1, \ldots, N$):

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix} \quad ; \quad \begin{pmatrix} b_i^+ \\ b_i \end{pmatrix} = \mathcal{W}^+ \begin{pmatrix} a_i^+ \\ a_i \end{pmatrix} \quad . \tag{3}$$

The minimization of the total routhian $\mathcal{E}^\omega$,

$$\mathcal{E}^\omega = \mathcal{E} - \lambda\langle\Psi|\hat{N}|\Psi\rangle - \omega\langle\Psi|\hat{J}_x|\Psi\rangle, \tag{4}$$

leads to the HFB eigenvalue problem for the $2N \times 2N$ matrix:

$$\begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} U \\ V \end{pmatrix} E \quad , \tag{5}$$

which gives two $N \times N$ matrices U and V as eigenvectors and the diagonal matrix E of N eigenvalues which are the quasiparticle routhians (qpr), $E_{ij}{=}\delta_{ij} E_i^\omega$. The complete HFB spectrum is composed of pairs of opposite eigenvalues [27] and in Eq. (5), only one eigenvalue from each pair should be selected. The Hartree-Fock hamiltonian h and the pairing potential Δ are constructed from the density matrix ρ and the pairing tensor κ:

$$\begin{aligned} \rho &= V^* V^T \quad , \\ \kappa &= V^* U^T \quad , \end{aligned} \tag{6}$$

according to

$$\begin{aligned} h_{ij} &= T_{ij} + \textstyle\sum_{kl} V_{ikjl}\, \rho_{lk} - \lambda\delta_{ij} - \omega J_{ij} \quad , \\ \Delta_{ij} &= \tfrac{1}{2} \textstyle\sum_{kl} V_{ijkl}\, \kappa_{kl} \quad . \end{aligned} \tag{7}$$

In order to find a self-consistent solution of the HFB equation (5) we have adopted a method which relies on the simultaneous use of two different bases of single-particle states. The first one is the basis of functions $\phi_i(\boldsymbol{r})$ which converge to the eigenfunctions of the Hartree-Fock hamiltonian h and the second one is the canonical basis, i.e., the basis of eigenstates of the density matrix ρ. The iteration procedure is performed in the following way.

Suppose we start at some point with a set of orthogonal functions $\phi_i(\boldsymbol{r})$ and with the hamiltonian h in the coordinate representation. First, we perform one imaginary-time-step evolution of the set $\phi_i(\boldsymbol{r})$ using h as an evolution operator. The imaginary-time evolution [28] has already become a standard technique in the HF coordinate-space calculations. It ensures that as iterations proceed, the set $\phi_i(\boldsymbol{r})$ converges to the eigenfunctions of h with the single-particle routhians e_i^ω as eigenvalues, $h_{ij}{=}\delta_{ij}(e_i^\omega{-}\lambda)$.

Second, we calculate the matrix elements Δ_{ij} of the pairing potential and the diagonal matrix elements h_{ii} of the Hartree-Fock hamiltonian in the basis of the new (imaginary-time evolved) wave functions $\phi_i(\boldsymbol{r})$. As discussed above the matrix h_{ij} converges to the diagonal matrix

and therefore we can safely disregard its off-diagonal matrix elements during the iteration. On the other hand, for $\hbar\omega{\neq}0$ all the matrix elements Δ_{ij} are in general nonzero both during the iteration and *after* the convergence is obtained.

Third, we solve Eq. (5) to obtain the matrices U and V, the quasiparticle routhians E_i^ω as well as the matrices ρ and κ by using Eq. (6). A diagonalization of the density matrix,

$$\rho_{kj} = \sum_i n_i W_{ki} W_{ij}^+ \quad , \tag{8}$$

provides us with the occupation coefficients n_i and with the unitary transformation W which relates the basis $\phi_i(\boldsymbol{r})$ to the canonical-basis wave functions $\varphi_i(\boldsymbol{r})=\sum_j W_{ji}\phi_j(\boldsymbol{r})$.

Finally, we construct the HFB density matrix in the coordinate space

$$\rho(\boldsymbol{r},\boldsymbol{r}\,') = \sum_i n_i\, \varphi_i(\boldsymbol{r})\varphi_i(\boldsymbol{r}')^* \quad , \tag{9}$$

which is given as a single sum of products of the wave functions $\varphi_i(\boldsymbol{r})$. This fact is crucial for a numerically effective calculation of local Skyrme densities on the spatial mesh and then of various terms in the Hartree-Fock hamiltonian. In fact, at this point the density matrix has a form identical to that used in the HF+BCS method although it corresponds to an unrestricted HFB variation. At the expense of handling two sets of single-particle wave functions we are thus able to solve the HFB equations by using techniques which have already been well developed for the HF+BCS method.

For our purpose, the two-basis method has several advantages. First of all it allows us to use the existing techniques to obtain solutions of the cranked HF equations associated with a Skyrme interaction directly on a three dimensional mesh. These have been presented in refs. [29, 30] and have been applied to study the high spin properties of ^{24}Mg and ^{80}Sr. Because they do not rely on an expansion on a basis, they can describe with the *same* good accuracy the very different shapes that a rotating nucleus can take (some examples are shown in Fig. 7 of [30]).

Moreover, a separate treatment of the particle-hole and particle-particle channels becomes possible. Although there exist effective forces which have been shown to describe reasonably well both channels of interaction simultaneously,[2] we believe that the present knowledge of the pairing effective interactions is not as sophisticated as that concerning the mean-field. This is especially true as far as its properties relevant to situations of time-reversal symmetry breaking such as encountered in high spins physics are concerned. Treating in two steps the particle and the quasiparticle spaces, permits us to evaluate the gap matrix in the particle basis $\phi_i(\boldsymbol{r})$ with a different interaction than the one used in the cranked HF equation.

Our two-basis method provides also a more natural scheme for limiting the phase space than the truncation generated by a fixed basis. Because we are solving the HFB problem (5) directly in the cranked HF basis, its dimension N can be chosen much smaller than that needed for the accurate description of the HF orbitals $\phi_i(\boldsymbol{r})$. Similarly as in the phenomenological approaches [37] and based on our former experience, we limit it to orbitals for which the particle routhians e_i^ω do not exceed a given value $e_{\mathbf{max}}^\omega$. This value should be much larger than $\lambda+\Delta$, where Δ is the physical pairing gap. The results

[2]For instance the SkP Skyrme interaction [31] or the earlier and mathematically sounder global effective interaction proposed by Gogny [32, 33, 34, 35, 36]

presented below have been obtained with $e^{\omega}_{\max}=\lambda+5$ MeV. This leads to a dimension of the HFB matrix of the order of hundred, compared to typical dimensions of the cranked HF equations of the order of several thousand.

By applying the two-basis method we have circumvented the difficulties associated with the fact that the HFB hamiltonian has a spectrum unbounded from below in the coordinate representation. Therefore, a direct application of any variational method (e.g., of the imaginary-time method) is impossible. When spherical symmetry is enforced, the HFB problem becomes one-dimensional and its solutions can be obtained [31] by explicitly solving a differential Schrödinger-like equation. However this route seems to be difficult to take for deformed systems which require a three-dimensional treatment. In practice, we use the double representation inherent to the two-basis method, to filter those states from the unbounded HFB spectrum which are the most physically important.

2.2 THE SENIORITY PAIRING INTERACTION IN THE CRANKED BASIS

In the present study, we use the simplest possible pairing force: the seniority interaction. This force being compatible with the signature symmetry, we can separate the phase space in two subspaces of dimensions n_1 and n_2 ($n_1 + n_2 = N$) associated with opposite signatures. In the following, we denote respectively with latin (i.e. i) and hat-topped latin indices (i.e. $\hat{\imath}$) states in the positive and negative signature subspaces. Then the non-zero matrix elements of the seniority forces are

$$V_{i\hat{\jmath}k\hat{l}} = -G\langle\hat{\jmath}|\hat{\mathcal{T}}|i\rangle\langle\hat{l}|\hat{\mathcal{T}}|k\rangle \quad , \tag{10}$$

plus all those obtained from the antisymmetry conditions. In (10), $\hat{\mathcal{T}}$ stands for the time-reversal operator. This expression corresponds to the lowest-order truncation of the pairing matrix elements of a short range force. The pairing strength G is parametrized for neutrons (protons) as $G_N = g_N/(11 + N)$ ($G_Z = g_Z/(11 + Z)$), as was done in our preceding studies. We discuss later how to select the values of the two parameters g_N and g_Z.

According to a well established procedure [38], we consider the matrices U and V in the following block form

$$U = \begin{pmatrix} u & 0 \\ 0 & \tilde{u}^* \end{pmatrix} \quad ; \quad V = \begin{pmatrix} 0 & \tilde{v}^* \\ -v & 0 \end{pmatrix} \quad , \tag{11}$$

in which the first block has dimension n_1 and the second dimension n_2. This leads to simplifications for ρ and κ:

$$\rho = \begin{pmatrix} r & 0 \\ 0 & \tilde{r}^* \end{pmatrix} \quad ; \quad \kappa = \begin{pmatrix} 0 & k \\ -k^T & 0 \end{pmatrix} \quad ; \quad \begin{cases} r = \tilde{v}\tilde{v}^+ \\ \tilde{r} = vv^+ \\ k = \tilde{v}\tilde{u} \end{cases} \quad , \tag{12}$$

and for h and Δ:

$$h = \begin{pmatrix} h & 0 \\ 0 & \tilde{h}^* \end{pmatrix} \quad ; \quad \Delta = \begin{pmatrix} 0 & d \\ -d^T & 0 \end{pmatrix} \quad , \tag{13}$$

where the expressions for h, $\tilde{h}$ and d can be obtained by inserting Eqs. (12) in Eqs.(7). Then the HFB equations (5) reduce to the following N-dimensional problem:

$$\begin{pmatrix} h & d \\ d^+ & -\tilde{h} \end{pmatrix} \begin{pmatrix} u & \tilde{v} \\ -v & \tilde{u} \end{pmatrix} = \begin{pmatrix} u & \tilde{v} \\ -v & \tilde{u} \end{pmatrix} \begin{pmatrix} E_i^\omega \delta_{ij} & 0 \\ 0 & -E_{\hat{i}}^\omega \delta_{\hat{i}\hat{j}} \end{pmatrix} \quad . \tag{14}$$

This last equation specifies our definition of the quasiparticle routhians (qpr) assuming that the eigenvectors of the diagonalization problem are ordered according to *decreasing* eigenvalues (n_1 first, n_2 last). The first n_1 eigenvectors are associated with the positive signature. The last n_2 eigenvectors are associated with the negative signature and the corresponding eigenvalues are opposite to the negative-signature qpr's. In particular, following the discussion in ref. [39] concerning the parity of the number of particles in the BCS state, we do not consider the signs of the eigenvalues to decide which qpr's are of a given signature.

In a similar manner, to study one-quasiparticle or two-quasiparticle states, we exchange the U and V components of eigenvectors according to the following procedure. First, we choose a given configuration by selecting the label i of the wave function $\phi_i(\boldsymbol{r})$ upon which the quasiparticle excitation is to be constructed. Then we scan the ith line in the matrix $\begin{pmatrix} u & \tilde{v} \\ -v & \tilde{u} \end{pmatrix}$ looking for the largest component to determine the column (i.e. the qpr) for which the exchange of the U and V components must be done. We can also determine whether this particular quasiparticle excitation is predominantly of the particle or of the hole type; in the former (latter) case the largest component is located in the u or $\tilde{u}$ (v or $\tilde{v}$) blocks. We have found this procedure more stable than that using the values of qpr's to select quasiparticle excitations. Indeed, during the course of the HFB iterations, the displacement of the Fermi level necessarily associated with the creation of one or two quasiparticles makes it difficult to recognize a given configuration solely on the basis of the value of its qpr.

2.3 THE LIPKIN-NOGAMI PRESCRIPTION

Although the HFB equations contain most of the ingredients essential for the understanding of the physics of fast rotating nuclei, they present a significant weakness inherent to their mean-field nature: for specific values of the angular velocity, they predict phase transitions which, in principle, should not occur in a finite system such as the nucleus. As we will show, such transitions generate characteristic behaviours in the evolution of the moment of inertia versus angular velocity which are incompatible with present data. They correspond to a sudden breakdown of neutron or proton pairing correlations and are associated with a poor description of particle-number symmetry breaking in situations of small particle-number fluctuations. To cure this deficiency while retaining the quality and

the simplicity of a mean-field description, the best approach would be a variation after projection (VAP) on correct particle number [27]. Because it appeared too difficult to implement it in this first study, we have adopted the approximate projection method proposed by Lipkin and Nogami [24, 25, 26]. The associated equations which we recall below have been tested to provide a good numerical approximation of the VAP in situations where both the HFB and the BCS equations predict a collapse of the pairing correlations. (See the recent studies of model systems without [40, 41] and with rotation [42], and the references cited therein.)

The prescription of Lipkin-Nogami amounts to modify the energy $\mathcal{E}$ (or the total routhian $\mathcal{E}^\omega$ in case of cranked HFBLN method) by adding the second-order Kamlah [43] correction:

$$\mathcal{E} \rightarrow \mathcal{E} - \lambda_2 \langle \Delta \hat{N}^2 \rangle \quad , \tag{15}$$

where $\langle \hat{O} \rangle$ denotes the expectation value $\langle \Psi | \hat{O} | \Psi \rangle$. The coefficient λ_2 is given by:

$$\lambda_2 = \frac{\langle \hat{H}(\Delta \hat{N}^2 - \langle \Delta \hat{N}^2 \rangle) \rangle - \langle \hat{H} \Delta \hat{N} \rangle \langle \Delta \hat{N}^3 \rangle / \langle \Delta \hat{N}^2 \rangle}{\langle \Delta \hat{N}^4 \rangle - \langle \Delta \hat{N}^2 \rangle^2 - \langle \Delta \hat{N}^3 \rangle^2 / \langle \Delta \hat{N}^2 \rangle} \quad . \tag{16}$$

For the HFB state, the moments of the operator $\Delta \hat{N} = \hat{N} - \langle \Delta \hat{N} \rangle$ which appear in the definition of λ_2 are given by [44]:

$$\left\{ \begin{array}{l} \langle \Delta \hat{N}^2 \rangle = 2 \, \mathrm{tr} \, [\chi] \\ \langle \Delta \hat{N}^3 \rangle = 4 \, \mathrm{tr} \, [\gamma \chi] \\ \langle \Delta \hat{N}^4 \rangle = 3 \langle \Delta \hat{N}^2 \rangle^2 + 8 \, \mathrm{tr} \, [\chi (1 - 6 \chi)] \end{array} \right. \quad ; \quad \left\{ \begin{array}{l} \chi = \rho (1 - \rho) \\ \gamma = 1 - 2 \rho \end{array} \right. \quad , \tag{17}$$

and

$$\left\{ \begin{array}{rl} \langle \hat{H} \Delta \hat{N} \rangle & = 2 \, \mathrm{tr} \, [h \chi] - \Re \, \mathrm{tr} \, [\Delta \kappa^* \gamma] \\ \langle \hat{H} (\Delta \hat{N}^2 - \langle \Delta \hat{N}^2 \rangle) \rangle & = 4 \, \mathrm{tr} \, [(h \gamma + v_{HF}\{\chi\}) \chi] - \Re \, \mathrm{tr} \, [\Delta \kappa^* (1 - 8 \chi)] \\ & \quad - \mathrm{tr} \, [v_P \{\gamma \kappa\} (\gamma \kappa)^*] \end{array} \right. \quad , \tag{18}$$

where the symbol $\mathrm{tr}\,[a]$ stands for the trace of the matrix a and $\Re$ denotes the real part. The mean fields $v_{HF}\{\chi\}$ and $v_P\{\gamma\kappa\}$ are the HF potential and the pairing potential calculated with the densities χ and $\gamma\kappa$, respectively:

$$v_{HF}\{\chi\}_{ij} = \sum_{kl} V_{ikjl} \chi_{lk} \quad ; \quad v_P\{\gamma\kappa\}_{ij} = \frac{1}{2} \sum_{kl} V_{ijkl} (\gamma\kappa)_{kl} \quad . \tag{19}$$

A consistent application of the Lipkin-Nogami prescription requires in principle using the full effective interaction in Eqs. (19). In the present study we calculate λ_2 by using only the seniority pairing interaction. However, in (18) the effects of the Skyrme interaction are still taken into account by the contributions containing the HF hamiltonian h. This is consistent with all the other applications of the Lipkin-Nogami prescription performed up to date. The fact that particle-number mixing is directly related to the existence of an

interaction in the particle-particle channel may be considered as a justification for such a procedure. Admittedly, further studies of this question are needed.

Assuming that the quasiparticle vacuum $|\Psi\rangle$ is a self-consistent solution, one may derive another formula for λ_2 which gives the same value as (16) at the end of the iteration procedure. In fact, this approach is usually taken in applications, because it gives λ_2 in terms of the two-body interaction only. For the case of the seniority pairing interaction such explicit expressions are given in refs. [26] and [42] without and with time-reversal symmetry breaking, respectively.

The modification of the HFB equations associated with the Lipkin-Nogami prescription is obtained by a restricted variation of $\lambda_2\langle\Delta\hat{N}^2\rangle$, namely, λ_2 is not varied although its value is calculated self-consistently using (16). Based on Eq. (17), this leads [26] to the modification of the HF hamiltonian, $h \to h - 2\lambda_2\gamma$, while the pairing potential Δ is unchanged. In the present study we have used this method to study ^{192}Hg, ^{194}Hg and ^{194}Pb. However, as noted in ref. [19], one may use an equivalent form of $\langle\Delta\hat{N}^2\rangle$=2tr $[\kappa^+\kappa]$, which leads to $\Delta \to \Delta - 4\lambda_2\kappa$ and leaves h unchanged. In this way, a better numerical stability of the HFBLN equations can be obtained [19]. We have also investigated an intermediate prescription:

$$h \to h - \lambda_2\gamma \quad ; \quad \Delta \to \Delta - 2\lambda_2\kappa \quad , \tag{20}$$

which results from inserting the explicit form of the particle-number operator (N_{ij}=δ_{ij}) only after the variations over ρ and κ are performed. Such a prescription also turns out to be numerically stable and was used to study ^{190}Hg.

3 Results

The calculations reported below have been performed using the SkM* parametrization [45] of the Skyrme force and the seniority pairing interaction as discussed in sec. 2.2. The method of solution of the cranked HF equations, which requires breaking of the time-reversal symmetry, has been discussed for the Skyrme interaction in refs. [29, 30]. The single-particle wave functions are discretized on a spatial rectangular mesh of points spaced by Δx=Δy=Δz=1fm. The parity and signature symmetries are assumed to be conserved, which allows us to solve the equations by using only points in space which have positive values of all three coordinates.

Although the code does not enforce it, the self-consistent solutions that we have obtained deviate little from axial symmetry: in all calculations the triaxiality angle γ never exceeds $\pm 0.2°$. The average value of the projection of angular momentum on the axis perpendicular to the symmetry axis J_0 is constrained while that of the quadrupole moment Q is unconstrained. In this way, the self-consistent quadrupole moment of the SD minimum is found for each value of the angular momentum and the evolution of Q is obtained as function of J_0.

We use a quadratic constraint on the angular momentum and therefore we are able to select values of J_0 along the rotational band equal to even integers. The Lagrange

multiplier ω required to obtain a given value of J_0 is interpreted as the angular velocity. Due to self-consistency the second moment of inertia $\mathcal{J}^{(2)}$, defined as

$$\mathcal{J}^{(2)} = \frac{\partial J_0}{\partial \omega}, \tag{21}$$

can be expressed in terms of the first derivative of the energy (2) with respect to ω,

$$\mathcal{J}^{(2)} = \frac{1}{\omega}\frac{\partial \mathcal{E}}{\partial \omega}. \tag{22}$$

Neglecting a weak dependence on ω of the Lagrange multipliers λ associated with proton and neutron numbers, one can also express the angular momentum as the first derivative of the total routhian $\mathcal{E}^{\omega}$, Eq. (4),

$$J_0 = -\frac{\partial \mathcal{E}^{\omega}}{\partial \omega}. \tag{23}$$

Within the same approximation one therefore obtains an alternate formula for the second moment of inertia:

$$\mathcal{J}^{(2)} = -\frac{\partial^2 \mathcal{E}^{\omega}}{\partial \omega^2}. \tag{24}$$

Because formulae (21) and (22) involve a first order derivative, they are numerically more stable than (24). Moreover, formula (21) which uses the average value of a one-body operator is easier to handle than (22) which depends on the two-body interaction. We have found that an accurate determination of $\mathcal{J}^{(2)}$ requires a high level of convergence. In order to make connection with the experimental method for determining the second moment of inertia we have also calculated $\mathcal{J}^{(2)}$ according to:

$$\mathcal{J}^{(2)} = \frac{4\hbar^2}{E_{I+2} - 2E_I + E_{I-2}}, \tag{25}$$

where E_I is the total energy $\mathcal{E}$ obtained by constraining the average value of the cranking angular momentum to even integers, i.e., $J_0{=}I$.

In practice we have to perform about 200 iterations (or 300 in the crossing regions) with an imaginary time-step $\delta t{=}0.015\hbar/\mathrm{MeV}$. Only then do we obtain the second moments of inertia calculated from (21) and (25) equal up to 1%.

At this point one should stress an important difference between the interpretation of quasiparticle routhians (qpr's) in the HF and the Nilsson-Strutinsky (NS) approaches. In both cases, the value of the angular momentum J_0 is the sum of contributions from individual quasiparticle states, $J_0{=}\sum_i j_i$, where j_i are the individual alignments, i.e., the average values of the cranking angular momentum $\hat{J}_x$ in the quasiparticle states. Therefore, the second moment of inertia (21) is also a sum of contributions from individual quasiparticle states, equal to the first derivatives of alignments with respect to ω. On the other hand, the NS individual alignments are equal to the opposite of the first derivatives of the NS qpr's, and hence their contributions to $\mathcal{J}^{(2)}$ are given by the second derivatives

of qpr's. This is no longer true for the HFB qpr's because the HF mean field *depends self-consistently* on the angular velocity (cf. discussion in ref. [20]). Only the *total* values of the angular momentum J_0 and of the second moment of inertia $\mathcal{J}^{(2)}$ are equal to the opposite of the first and the second derivatives of the *total* routhian, Eqs. (23) and (24), respectively. They have, however, no direct relations with the sums of the first and the second derivatives of qpr's with respect to ω. This fact should be kept in mind when analyzing the diagrams of the HFB or HFBLN qpr's. In particular, the changes in $\mathcal{J}^{(2)}$ caused by a quasiparticle excitation cannot not be simply inferred from these diagrams.

3.1 EFFECT OF DIFFERENT TREATMENTS OF PAIRING CORRELATIONS

Figure 1 presents a comparison of the second moment of inertia $\mathcal{J}^{(2)}$ calculated within the cranked HF, HFB and HFBLN approximations for the nucleus ^{192}Hg.

The HF moment of inertia[3] keeps an almost constant value ($\approx 115\hbar^2\mathrm{MeV}^{-1}$) versus angular velocity. A similar result obtained within the WSNS method is reported in ref. [22]. This constancy is in contradiction with the data which show a steady increase of $\mathcal{J}^{(2)}$ from 90 to $135\hbar^2\mathrm{MeV}^{-1}$ over the range $100\mathrm{keV}\leq\hbar\omega\leq450\mathrm{keV}$. One is therefore led to conclude that in the mercury region pairing correlations play an important role in the superdeformed high-spin states. The increase of $\mathcal{J}^{(2)}$ would then be at least partially attributed to a reduction of the superfluidity as the magnitude of the time-reversal-breaking cranking field grows.

The HFB results obtained with a seniority force $g_N = g_Z$=15.5MeV do indeed display an increase of $\mathcal{J}^{(2)}$ (Fig. 1) which is however too rapid at low rotation frequencies. Despite a value of $\mathcal{J}^{(2)}(0)\equiv\mathcal{J}^{(2)}(\hbar\omega=0)$ which is lower than indicated by experiment, the moment of inertia becomes larger than the experimental values in less than ten units of angular momentum. In addition, the HFB curve presents two sudden drops at $\hbar\omega$=250keV and 350keV. These two accidents in the $\mathcal{J}^{(2)}$ curve are due to the collapses of the proton and neutron pairing correlations. This is shown by Fig. 2 which displays the evolution versus $\hbar\omega$ of the proton and neutron pairing contributions to the total energy defined by:

$$\mathcal{E}^P_\tau(\hbar\omega) = -\mathrm{tr}\left[\Delta_\tau\kappa^*_\tau\right] \quad , \tag{26}$$

where the index τ refers to neutrons (N) or protons (Z). The fact that the proton pairing disappears first and the neutron pairing later is related to the magnitude of the pairing correlations at $\hbar\omega$=0 which are weaker for protons than for neutrons. This in turn reflect the corresponding sizes of the SD shell effects.

Fig. 3 gives the evolution of the neutron and proton single-particle energies versus quadrupole deformation in the neighbourhood of the SD well. One sees that for the SkM*

[3]There is a $2\hbar^2\mathrm{MeV}^{-1}$ reduction of the value of $\mathcal{J}^{(2)}$ as compared with the calculations of ref. [20] which have been performed with Δx=0.8fm. It measures the absolute inaccuracy of the present calculation (performed with Δx=1fm) in replacing the differential operators of the Skyrme functional and of the angular momentum by a finite-difference expression on the spatial mesh.

interaction, the proton magic gap at Z=80 is large and dominates the neutron shell effect at N=112 which occurs at a slightly larger deformation. WSNS calculations also find that this proton gap in the single-particle spectrum is larger than the neutron gap. As a consequence, at $\hbar\omega$=0 the proton pairing correlations are weaker than neutron ones and tend therefore to disappear first. Once the pairing correlations have vanished, the HFB moment of inertia $\mathcal{J}^{(2)}$ becomes identical to that of the HF method.

The introduction of an approximate treatment of particle number projection by the Lipkin-Nogami method modifies the behaviour of $\mathcal{J}^{(2)}$ and $\mathcal{E}^P_\tau$ as function of $\hbar\omega$. Because the projection always leads to an increase of pairing correlations (cf. ref [46]), we had to lower the pairing strengths to $g_N = g_Z = 14$MeV so as to obtain a moment of inertia close to that found with the HFB method at $\hbar\omega$=0. Fig. 2 shows that despite this reduction, the proton pairing energy $\mathcal{E}^P_Z(0)$ is significantly increased over the HFB value while $\mathcal{E}^P_N(0)$ is much less affected. This reflects another characteristics of the particle-number projection which induces larger relative modifications whenever the pairing correlations are weak, i.e., when the particle shell effects are large.

Within the HFBLN method the pairing energies decrease smoothly with the angular velocity (Fig. 2). The spurious sudden phase transitions disappear and the calculations predict a regular increase of the moment of inertia without any discontinuity (Fig. 1). Still one notes that at $\hbar\omega$=0 the moment of inertia is smaller than the value suggested by an extrapolation of the experimental data. Since we consider this work as a first step towards a more complete analysis of the effective interaction in the particle-particle channel, we have chosen to further renormalize the pairing strength so as to have a value of $\mathcal{J}^{(2)}(0)$ in agreement with experiment. This is obtained by the reduction of both pairing intensities to the values of $g_N = g_Z = 12.6$MeV. In all likelihood, such a modification lies within the present domain of uncertainty of a pairing force defined entirely on the basis of static properties such as quasiparticle energies at ground state or deformation energy curves. Dynamical properties such as the moment of inertia $\mathcal{J}^{(2)}$ will certainly introduce stronger constraints.

With these reduced values of g_τ, we find that at $\hbar\omega$=0 the neutron and proton pairing gaps of ^{192}Hg are equal to Δ_N=0.557MeV and Δ_Z=0.647MeV, respectively. The evolution of pairing energies versus $\hbar\omega$ (Fig. 2) shows an interesting feature: their rate of decrease versus $\hbar\omega$ is reduced together with their values. This yields larger pairing correlations at high frequencies and hence a slower increase of $\mathcal{J}^{(2)}$ versus $\hbar\omega$ in better agreement with data (Fig. 1). At the highest spins reached in the present study, the pairing correlations are still present for all the nuclei considered. For instance, the pairing energies $\mathcal{E}^P_N$ and $\mathcal{E}^P_Z$ in ^{194}Pb are at J_0=52$\hbar$ still of the order of 0.5MeV (see Fig. 4).

Had we been interested in a purely phenomenological analysis of data, we could probably have improved the agreement by introducing values of g_N different from those of g_Z while keeping the value of $\mathcal{J}^{(2)}(0)$ consistent with the experimental data. On the other hand, in our opinion the relative importance of the neutron and proton pairing should be ultimately determined by the isospin symmetry. Unfortunately, this symmetry cannot be straightforwardly implemented within a seniority interaction which is by defined separately for neutrons and protons. We have therefore chosen to defer to further studies

such an analysis which will involve a short-range pairing force. All the results, discussed hereafter have been obtained with the the pairing strengths $g_N = g_Z = 12.6$MeV.

3.2 HIGH-SPIN PROPERTIES OF GROUND-STATE SUPER-DEFORMED BANDS

In this section we present results for the ground superdeformed bands of the ^{190}Hg, ^{192}Hg, ^{194}Hg and ^{194}Pb nuclei. Fig. 5 shows the evolution of their charge quadrupole moments Q_c versus $\hbar\omega$. The results for the four nuclei are qualitatively different. The curves for ^{192}Hg and ^{194}Hg display an expected behaviour (see also Fig. 3 in ref. [17]): after a small increase that can be attributed to the diminishing of pairing correlations, the usual effect of quantum rotations [47] takes over and leads to a decrease of Q_c. For ^{194}Pb the deformation of the minimum of the SD well at J_0=0 is larger than in the mercury isotopes, even when the 4% effect on Q_c associated with the two additional neutrons is taken into account. This can be explained by considering two characteristics of the Z=82 subshell effect (see Fig. 3): first it is shifted to slightly larger deformation than the Z=80 one; second it is weaker, so that the neutron N=112 shell effect acts more efficiently and pulls the deformation to larger values. Similar properties are visible in the particle proton spectrum obtained with the WSNS method (see Fig. 6 of ref. [17]). Another specificity of the evolution of Q_c for ^{194}Pb is its constant growth versus $\hbar\omega$.

The curve for ^{190}Hg displays two distinct patterns. At low angular velocities ($\hbar\omega \leq 325$keV) the behaviour is similar to that of the other two Hg isotopes. Then occurs a neutron two-quasiparticle alignment (see below) so that the neutron pairing is reduced (see Fig. 4). This alignment leads to a further reduction of the quadrupole moment as discussed in [47].

These calculated variations of Q_c are smaller than the present level of accuracy of the experiments which are still consistent with unchanging quadrupole moments [48, 49]. We hope that coming improvements in the γ-ray detectors will allow the observation of such fine differences in the behaviour of the quadrupole moment versus $\hbar\omega$. These variations are however sufficiently large to significantly modify the dependence of single-particle routhians on $\hbar\omega$. This is so because deformation effects on single-particle states are in general stronger than those induced by rotation. Fig. 6 presents the single-particle routhians in ^{190}Hg calculated along the path of self-consistent quadrupole moments. One can see that after the crossing the $\hbar\omega$-dependence of the routhians is modified, and more pronounced because of faster changes of the deformation.

Fig. 7 shows the single-particle routhians of ^{192}Hg. There is a large proton shell effect for Z = 80 and weaker neutron ones for N=104, 110, 112 and 118. There exists also a weaker proton shell effect for Z=82. This spectrum looks much like that obtained within the WSNS [22, 23] approach. However, we note some small deviations which may explain some of the features that we discuss below.

In the following, we label the single-particle and quasiparticle routhians by their dominant components in the asymptotic Nilsson basis. Let us recall that this labelling is mostly useful to attribute names to the discussed orbitals. Indeed, the dominant compo-

nents have sometimes weights as low as 20% (see ref. [50] for a detailed analysis).

In the neutron spectrum, the SkM* force places the intruder orbitals $\nu[770]_{1/2}$, $\nu[761]_{3/2}$ and $\nu[752]_{5/2}$ about 0.8MeV lower than does the WSNS approach (with respect to the rest of the spectrum). On the other hand, the proton spectrum is very similar. The only noticeable difference is the existence in our calculation of a bunching of three levels at the Fermi surface which leaves the $\pi[651]_{3/2}$ intruder level isolated with small gaps at Z=72 and Z=74. In the WSNS spectrum, these four levels are more evenly spread over 0.8MeV. The effect of the change of deformation between ^{190}Hg and ^{192}Hg can be seen by comparing the proton single-particle routhians in Figs. 6 and 7. At J_0=0 the three orbitals below the Fermi level are more spread in ^{190}Hg than in ^{192}Hg and the Z=74 gap is less visible. This spectrum is therefore more similar to that in ref. [17].

Figure 8 shows the evolution of the second moment of inertia $\mathcal{J}^{(2)}$ for ^{192}Hg, ^{194}Hg and ^{194}Pb. The general behaviour of the data [5, 7, 8, 13] is correctly reproduced, in particular the apparition of a plateau at large $\hbar\omega$ is obtained. We also reproduce the relative positions of the curves for the three nuclei: ^{194}Hg lies above ^{192}Hg which itself is above ^{194}Pb. Presently we have no explanation for the slightly too rapid increase of the HFBLN moment of inertia. An analogous deficiency is also present in the recent WSNS LN calculations [19] for ^{194}Hg. However, since the results can be very sensitive to moderate changes of the pairing force, we think that it could be attributed to a slight imbalance between the neutron and proton strengths. The fact that we predict a too early occurrence of the plateau for ^{192}Hg and ^{194}Hg and the right one for ^{194}Pb supports such a conjecture.

Our calculations show that the values of $\mathcal{J}^{(2)}$ are not simply related to the deformation, contrary to what would occure for deformed rigid bodies. For instance, the nucleus ^{194}Pb which, among the studied nuclei, has the largest quadrupole moment, has the smallest moment of inertia. This shows to what extent the magnitude of a dynamic quantity such as $\mathcal{J}^{(2)}$ is unrelated with a static property such as Q_c. Our finding for ^{194}Pb is also in agreement with the general observation that for SD nuclei the rate of $\mathcal{J}^{(2)}$ variation versus $\hbar\omega$ is correlated with the occupation of the intruder orbital $\pi[642]_{5/2}$.

The calculated and experimental [23] second moments of inertia of ^{190}Hg (Fig. 9) grow also slowly as a function of the angular momentum until $\hbar\omega$=325keV where the calculation gives a peak due to the two-quasiparticle alignment associated with the $\nu[761]_{3/2}$ orbital, see Fig. 10. Note that it is precisely at this frequency that the single-particle routhian[4] $\nu[761]^{-}_{3/2}$ crosses the Fermi level (Fig. 6). This illustrates the fact that in the HFB theory the occupation probabilities are not directly determined by the eigenvalues of the mean-field hamiltonian. Although the experimental error is still large, the last point of the data suggests that a crossing will happen at a slightly higher angular velocity.

[4]The superscripts $+$, $-$ or $\pm$ at the Nilsson labels denote the signatures of orbitals

3.3 QUASIPARTICLE ROUTHIANS IN THE HG REGION

In the nuclei which differ from ^{192}Hg by no more than two nucleon units, 30 SD bands have already been observed (in ^{191}Au, $^{190-4}$Hg, $^{192-4}$Tl and ^{194}Pb [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13] From this information some general features have already become apparent.[5]

- It appears that pairing correlations are always playing a significant role. Except for two bands in ^{192}Tl, the $\mathcal{J}^{(2)}$ of all considered SD bands is growing.
- The nuclei having a comparable content of intruder states have similar slopes of $\mathcal{J}^{(2)}$ as function of $\hbar\omega$. The fact that this is independent of whether the nuclei are odd or even is an additional indication that dynamic pairing correlations (as described for instance by particle number projection) are present and are at least as important as the static ones contained in a simple HFB description.
- As in the rare earth region, there are also specific trends associated with the content of the proton or neutron intruder-state configuration. For instance, one can group several SD bands into a "family" associated with the ground SD band in ^{192}Hg. These bands have the fastest growing second moment of inertia $\mathcal{J}^{(2)}$. Among them there are several examples of pairs of identical bands.
- Recently another family associated with two SD bands in ^{193}Tl has emerged [11]. It includes mostly bands assumed to have the $\pi[642]_{5/2}$ orbital blocked. One can also add to this family the ground SD band in ^{191}Hg which is interpreted as having the $\nu[761]_{3/2}$ orbital blocked. If this orbital assignments are correct, this would indicate that the effects of proton and neutron intruder states are of a similar magnitude.
- A few bands, one recently discovered in ^{193}Hg [9] and two in ^{192}Tl [2, 11], display a markedly different behaviour. The latter two can be explained by a blocking of two (neutron and proton) intruder states at the same time. Similar bands have also been observed in ^{195}Tl [11].

We first consider the HFBLN quasiparticle routhians for ^{192}Hg (Figs. 11 and 12). Because we are going to discuss results for neighbouring nuclei, we have labeled the routhians (at $\hbar\omega$=0) not only with their dominant Nilsson configurations but also with a letter p or h to indicate whether they are built on a particle or a hole configuration. If a nucleus is related to ^{192}Hg by an addition of particles, the Fermi level will raise. One expects that the qpr's built on hole states will be pushed up while those built on particle states will go down. The opposite effect will occur when the nucleus is obtained by a subtraction of nucleons.

[5]Because this is a rapidly evolving domain of physics, there is unfortunately no consensus on the labeling of the bands in the available literature. Sometimes signature partners are denoted with consecutive numbers, sometimes with the same number and alphabetical (a and b) indices. We shall therefore avoid such labeling and when necessary, refer to the bands by what seems to be their most probable structure according to today's models.

In the proton diagram (Fig. 11), the qpr associated with the $\pi[642]_{5/2}$ orbital is well separated from the other ones. It displays a rather gentle alignment pattern and a very small signature splitting. This is in agreement with the observation that in all Tl isotopes, the bands can be sorted in pairs of signature partners. Moreover, the fact that their moment of inertia $\mathcal{J}^{(2)}$ is always growing less rapidly than that of ^{192}Hg is consistent with having one intruder orbital blocked.

Experimental routhians can be extracted from the information for the two bands of ^{193}Tl by taking ^{192}Hg as a reference and making reasonable assumptions for the spins. They show a decrease of this particular qpr of about 0.4MeV in the range of angular velocities of $110 \leq \hbar\omega \leq 360$keV and a maximal signature splitting of 30keV. In our calculations we find 0.6MeV and 80keV, respectively, for these two quantities. A similar analysis of the $\pi[642]_{5/2}$ qpr in ^{194}Pb leads to smaller numbers: 0.52MeV and 50keV. It therefore seems that our calculations predict a slightly too large proton alignment. This could explain why the HFBLN moments of inertia (Fig. 8) increase somewhat faster than the experimental data.

The qpr's associated with the three hole levels $\pi[532]_{3/2}$, $\pi[530]_{1/2}$ and $\pi[411]_{1/2}$ are located around 1MeV. For lighter neighbouring elements, these qpr's become the lowest ones and replace in the qpr spectrum those built on the particle orbital $\pi[642]_{5/2}$. In ^{191}Au our calculation would therefore predict three bands close in energy. The one built on $\pi[411]_{1/2}$ would not have an easily detectable partner because of the strong signature splitting. It is tempting to say that this is the band which has already been observed. The other two result from a strong interaction between the levels $\pi[532]_{3/2}$ and $\pi[530]_{1/2}$, which pushes down the qpr's $\pi[532]^{+}_{3/2}$ and $\pi[530]^{-}_{1/2}$ of opposite signatures.

In this respect, our calculation differs slightly from that using the WSNS method. Indeed, because the particle routhian built on the orbital $\pi[532]_{3/2}$ is lower in the spectrum of ref. [4], there is less interaction with the one built on $\pi[530]_{1/2}$. Since this orbital has a large signature splitting, one should then in principle expect to find only one other band without a partner. However, we note that the signature splitting of levels (see for instance $\pi[411]_{1/2}$ in Fig. 3 of ref. [4]) in the WSNS approach is smaller than the one found in the present work. Therefore their predicted signature partners are never very far in energy. In addition, the negative-signature intruder orbital $\pi[651]^{-}_{3/2}$ obtained in ref. [4] seems to interact earlier ($\hbar\omega \approx 250$keV) with $\pi[411]^{-}_{1/2}$. It crosses it and appears at the Fermi surface at $\hbar\omega$=0.300keV. In our calculation, until $\hbar\omega$=410keV, the $\pi[651]^{-}_{3/2}$ state is still not favoured as compared to the orbitals $\pi[411]^{-}_{1/2}$ and $\pi[532]^{\pm}_{3/2}$. Further experiments on gold isotopes may certainly help clarify this situation.

Let us now consider the qpr spectrum for neutrons (Fig. 12). At J_0=0 one first finds a group of three levels. Two are of the particle type, $\nu[512]_{5/2}$ and $\nu[624]_{9/2}$, and one of the hole type $\nu[642]_{3/2}$. Further up there is a group of four levels. Among them there are two routhians built on intruder orbitals: the particle-type $\nu[752]_{5/2}$ and the hole-type $\nu[761]_{3/2}$. Because of a strong interaction between these two intruder routhians, they almost immediately exchange their character when $\hbar\omega$ increases. In particular, it seems more appropriate to assign the steep downgoing branch which comes out of the qpr labeled

$\nu[752]_{5/2}$ to the orbital $\nu[761]_{3/2}$. At this point, we will only justify this affirmation by noting that the signature splitting of the latter routhian is larger than that of the former one (see Fig. 7) because it has a smaller value of K. Later, we will analyze this point in more details when comparing the neutron qpr spectra of the four mercury isotopes studied in this work.

If we try to extrapolate from this spectrum that of ^{191}Hg, we expect that the most interesting configurations will be those associated with the hole-type qpr's: those of the two signature-partner states of $\nu[642]_{3/2}$ and the negative-signature down-going state $\nu[761]^{-}_{3/2}$. We note that for $\hbar\omega$>300keV the latter qpr is the least excited one. Moreover, in ^{190}Hg the same state is the least excited already at $\hbar\omega$=120keV (Fig. 10). One can therefore infer that the corresponding crossing will happen in ^{191}Hg at an intermediate angular velocity. Since the SD bands are essentially fed at high spins, it is natural to expect the $\nu[761]^{-}_{3/2}$ band to be the most populated. Then should come two bands with moderate signature splitting associated with $\nu[642]^{\pm}_{3/2}$. This corresponds well to the experimental situation. The extraction of the experimental qpr's for the two signature-partner bands shows an approximate overall decrease of 150keV with a maximal splitting of about 40keV over the range of $150\leq\hbar\omega\leq380$keV. For these two numbers we find 330keV and 100keV, respectively. Therefore, as was the case for protons in ^{193}Tl, we find also a neutron alignment which is slightly too large.

We consider now the heavier isotope ^{193}Hg. A hole state such as $\nu[642]_{3/2}$ will now become higher than the two particle states $\nu[512]_{5/2}$ and $\nu[624]_{9/2}$. On the latter orbital two SD bands with a negligible signature splitting can be built. Candidates for these bands exist in the experimental data. Similarly, there should also be a band built on the $\nu[512]^{+}_{5/2}$ qpr. This band should be very similar to the two previous ones because of the strong similarity of their qpr's which remain almost parallel to each other. This has also been observed. In addition our diagram shows that the negative-signature orbital $\nu[512]^{-}_{5/2}$ interacts strongly with $\nu[761]^{-}_{3/2}$. Such a phenomenon has precisely been seen in the experiment [51, 5, 6]. Moreover, recently a candidate for the $\nu[761]^{+}_{3/2}$ band has been observed [9] with a reduced $\mathcal{J}^{(2)}$ which is compatible with an upbending behaviour of the associated qpr, as is visible in our qpr spectrum. The $\hbar\omega$ value for the crossing is measured to be equal to 250keV and compares favourably with the value of 200keV obtained in our calculations.

Let us now pursue this discussion by considering in more details the evolution of the neutron qpr spectrum as function of the neutron number for the mercury isotopes. Fig. 13 includes selections of levels from the qpr spectra obtained for the ground SD bands of ^{190}Hg, ^{192}Hg and ^{194}Hg. We have also included the spectrum obtained by a calculation of ^{193}Hg treated as an *even* nucleus, using the fact that the number of particle of a BCS wave-function is only defined on the average. The qpr's shown in Fig. 13 for ^{193}Hg result from a calculation in which we have arbitrarily imposed that the average neutron number is equal to 113. This allows us to study the influence of the position of the Fermi level on the crossing of the negative-signature $\nu[512]_{5/2}$ states with the N=7 intruder states.

The qpr's shown in Fig. 13 are $\nu[642]_{3/2}$ and $\nu[761]_{3/2}$ for the holes states, and $\nu[512]_{5/2}$ and $\nu[752]_{5/2}$ for the particle states. To make the figure more readable, we have eliminated the qpr's associated with the hole states $\nu[505]_{11/2}$ and $\nu[640]_{1/2}$ which play no role in our discussion and the particle state $\nu[624]_{9/2}$. The latter qpr shows no sign of signature splitting. In all Hg isotopes, it remains parallel to the $\nu[512]^{+}_{5/2}$ orbital with an energy shift which decreases gradually from 150keV in ^{190}Hg to almost zero in ^{194}Hg. As mentioned above, two signature-partner bands in ^{193}Hg have been assigned to this particular orbital $\nu[624]_{9/2}$.

The ^{190}Hg qpr diagram shows that the single-particle dynamics is determined mostly by the alignment of the strongly signature-split orbital $\nu[761]_{3/2}$ whose negative-signature partner crosses the $\nu[642]_{3/2}$ at $\hbar\omega$=120keV, then becomes negative at $\hbar\omega$=300keV and generates an alignment at $\hbar\omega$=325keV. At this frequency, the experimental $\mathcal{J}^{(2)}$ indicates no alignment but the last available data point [23] suggests a possible crossing at a higher angular frequency. Moreover, we obtain a slightly too large slope of the second moment of inertia prior to the peak. Both facts suggest again that our calculations predicts an alignment faster than seen in the experiment.

From the separation of the qpr's, we estimate that the interaction between the ground SD band and the two-quasiparticle band is approximately 300keV. According to our diagram it seems also that a negative-parity band built on the $\nu[642]^{-}_{3/2}$ will become yrast beyond $\hbar\omega$=400keV.

In the qpr diagrams of ^{192}Hg, ^{193}Hg and ^{194}Hg (Fig. 13), there is a modulation of the interaction between the intruders $\nu[761]^{-}_{3/2}$ and $\nu[752]^{-}_{5/2}$, and the $\nu[512]^{-}_{5/2}$ orbital as the hole-type qpr's move up in the spectrum. In ^{194}Hg, the $\nu[761]_{3/2}$ is pushed so high by the displacement of the neutron Fermi level that despite its rapid descent, its negative-signature branch $\nu[761]^{-}_{3/2}$ does not interact with $\nu[752]^{-}_{5/2}$ before $\hbar\omega$=360keV. Had we pursued the calculation to higher spins, an extrapolation suggests that an interaction with the $\nu[512]^{-}_{5/2}$ would have occurred near $\hbar\omega$=440keV. It is interesting to see that in these four isotopes of mercury, the $\nu[752]^{+}_{5/2}$ curve displays precisely the upbending behaviour of the experimental routhian of the band recently discovered in ^{193}Hg [9]. Qualitatively speaking, one could then say that the SD band interaction observed in ^{193}Hg concerns the $\nu[761]^{-}_{3/2}$ and $\nu[512]^{-}_{5/2}$ states while the last SD band in the same nucleus is built on the $\nu[752]^{+}_{5/2}$ state. Of course, we must keep in mind that within the energy range of the order of the pairing gap around the Fermi level, one cannot distinguish between holes and particles. As shown in the qpr spectrum of ^{190}Hg (Fig. 10) the $\hbar\omega$=0 identity of the qpr's is rapidly lost if they happen to be close in energy and have large Coriolis coupling matrix elements, as is the case for $\nu[752]_{5/2}$ and $\nu[761]_{3/2}$.

The qpr spectrum of ^{193}Hg is intermediate between that of ^{192}Hg and ^{194}Hg. One sees that the lowering of the $\nu[761]_{3/2}$ is not large enough to induce an interaction at the values of $\hbar\omega$ where it has been observed. In our calculation the interaction only occurs at $\hbar\omega$=380keV. Nevertheless, there does not seem to be any need to invoke dynamical octupole correlations to explain the value of $\hbar\omega$ at which the band crossing occurs in ^{193}Hg [22]. This is also in line with the results of the Generator Coordinate Calculations

[52, 53] which find that a collective one-octupole-phonon SD band would be excited by approximately 1.7MeV with respect to the ground SD band, and therefore difficult to detect with presently available techniques. In fact, a mere 200keV up shift of the J_0=0 position of the $\nu[761]_{3/2}$ intruder state would certainly eliminate most of the discrepancies between our calculations and experiment. We will come back to this question in the concluding section.

The neutron qpr spectrum of ^{194}Pb is presented in Fig. 14. A comparison with the isotone nucleus ^{192}Hg (Fig. 12) shows the influence of the proton-induced polarization. According to the above discussion, because the Z=82 SD shell effect is weaker than the Z=80 one, the deformation of ^{194}Pb is larger. As a result (see for instance Fig. 3), the $\nu[752]_{5/2}$ orbital is approximately equidistant to $\nu[761]_{3/2}$ and $\nu[512]_{5/2}$ at $\hbar\omega$=0 (in ^{192}Hg, it is closer to $\nu[761]_{3/2}$). Now instead of two successive interactions, one observes a global interaction involving the three negative-signature levels for values of $\hbar\omega$ ranging from 150keV to 450keV. This behaviour so different from that observed in ^{192}Hg results from a mere 50keV shift of the $\nu[752]_{5/2}$ qpr away from the $\nu[761]_{3/2}$ orbital.

4 Summary and conclusions

In order to analyze nuclear structure at high angular momentum, we have constructed a cranked Hartree-Fock-Bogoliubov code. We solve the equations iteratively by performing in sequence the following operations. In the first one we evolve the single-particle wave functions by one imaginary-time step using the cranked Hartree-Fock mean field. In the second one we build the HFB matrix and solve the associated eigenvalue problem. After selecting the occupied quasiparticle states we compute the one-body density matrix and the pairing tensor. Then the eigenfunctions of the density matrix and the associated occupation probabilities are used to define the potential and the effective mass which enter the cranked Hartree-Fock mean field. This completes one iteration.

This method of solution which requires the simultaneous handling of two single-particle bases, allows an easier separation of the particle-hole and particle-particle (pairing) channels. It also permits a significant reduction of the size of the HFB problem. Since it is our feeling that the mean-field part of the effective force is reasonably well known (at least in the vicinity of the stability line), we plan to use this method to explore in more detail the pairing channel whose influence on the rotational properties of nuclei is expected to be important.

A HFB test calculation for the nucleus ^{192}Hg has shown the limitations of the mean-field method. At the angular velocities for which either proton or neutron pairing disappears , the dynamical moment of inertia displays abrupt decreases which are not compatible with the experiment. It is known that this deficiency results from a poor treatment of pairing correlations by the mean-field approach in the critical and subcritical regimes. It is also known that this can be improved by a variation after particle number projection (VAP). We have used the Lipkin-Nogami prescription (HFBLN) which provides a good approximation of the exact VAP. As expected, the HFBLN results for $\mathcal{J}^{(2)}$ do not display

spurious phase transitions and are in good qualitative agreement with data.

We have studied the ground superdeformed bands of the four nuclei ^{190}Hg, ^{192}Hg, ^{194}Hg and ^{194}Pb. The agreement is generally good. Using a single parameter for the strength of the pairing force, and adjusting it to reproduce the experimental dynamical moment of inertia at low frequency, we can obtain the slow upgoing behaviour of data including the appearance of a plateau around $\hbar\omega$=300keV. We also find that the $\mathcal{J}^{(2)}$ of ^{194}Pb is smaller than that of ^{192}Hg which itself is smaller than that of ^{194}Hg. An analysis of the quasiparticle routhians has shown that our spectrum is compatible with the single-particle structure of the SD well as it can be deduced from the present experimental knowledge based on 30 bands in nuclei which are close neighbours of ^{192}Hg. This includes the interesting band-interaction effect observed in ^{193}Hg.

Despite this good agreement, we have detected some weaknesses in our results. The most evident one is a slightly too fast alignment. It seems reasonable to assign this property to a too simple form of the pairing interaction. Several lines of improvements appear possible. First one could consider modifying the relative balance of the neutron and proton strengths. One can also study the effects coming from a more refined interaction such as for instance a density-dependent zero-range force.

It has also become apparent that a good description of data requires a very precise determination of the particle spectrum at $\hbar\omega$=0. We have seen that our spectrum differs from that obtained within the WSNS approach [17] as far as the positions of some neutron intruder states are concerned. The differences between the models may originate from small variations on the position of the intruder states at sphericity. Indeed any such difference will be emphasized by the large deformation associated with superdeformation. Another cause might be the value of the equilibrium deformation at the minimum of the SD well. Since we are often dealing with states which in the Nilsson diagram are rapidly up- or downgoing, a modification of the equilibrium deformation (of the order of 1e.b for Q_c) could explain the differences between our spectrum and that of ref. [17]. Since we have seen that the deformation of proton and neutron shell effects are slightly offset, a small modification of proton versus neutron pairing strengths could probably realize this effect. In fact, the uncertainty as to the exact magnitude of the deformation is only one more example stressing the importance of polarization effects on the high spin behaviour of nuclei: in this work, we have also discussed a case where a change in proton occupation modifies the behaviour of the neutron quasiparticle routhians.

Altogether the differences between various approaches in predicting the high-spin structure remain rather small, at least for those which also successfully describe collective properties at zero spin. Such differences could even be considered as being within the predictability range of the methods themselves. Nevertheless the challenge is there: the quality of present experimental information has introduced us into an era where much stricter requirements will be imposed on nuclear structure models.

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Figure Captions

Figure 1: The second moment of inertia $\mathcal{J}^{(2)}$ of the ground SD band of ^{192}Hg. The data (open circles) are taken from ref. [8]. The other curves correspond to the HF (solid line), HFB with g_τ=15.5MeV (triangles), HFBLN with g_τ=12.6MeV (solid circles) and HFBLN with g_τ=14MeV (solid squares) calculations.

Figure 2: Pairing contribution to the total energy of the ground SD band of ^{192}Hg. The curves correspond to the HFB with g_τ=15.5MeV (dashes), HFBLN with g_τ=12.6MeV (solid line) and HFBLN with g_τ=14.MeV (dots) calculations.

Figure 3: Nilsson diagram obtained by a quadrupole constrained HFBLN calculation for the nucleus ^{192}Hg at $\hbar\omega$=0. The deformation is measured by the charge quadrupole moment in e·b. The levels are indexed by their dominant asymptotic configuration. Positive- and negative-parity levels are drawn as solid and dot-dashed lines, respectively. The dotted line indicates the Fermi level. The arrows indicate the charge quadrupole moment of the SD minimum.

Figure 4: Proton (dashes) and neutron (solid line) pairing energies in MeV versus angular velocity for the ground SD bands.

Figure 5: Charge quadrupole moments in e·b versus angular velocity for the ground SD bands.

Figure 6: Single-particle routhians as function of the angular velocity for the ground SD band of the nucleus ^{190}Hg. The convention for the different (parity, signature) combinations is: $(+,+)$ solid line, $(+,-)$ dashed line, $(-,+)$ dot-dashed line, $(-,-)$ dotted line.

Figure 7: Same as in Fig. 6 for ^{192}Hg.

Figure 8: The second moments of inertia $\mathcal{J}^{(2)}$ of the ground SD bands of ^{194}Hg, ^{192}Hg and ^{194}Pb. Data for ^{194}Hg [22], ^{192}Hg [8] and ^{194}Pb [7] are indicated respectively by empty squares, circles and triangles. HFBLN results are drawn as dashed (^{194}Hg), solid (^{192}Hg) and dot-dashed (^{194}Pb) curves and solid symbols.

Figure 9: The second moment of inertia $\mathcal{J}^{(2)}$ of the ground SD band of the nucleus ^{190}Hg. Data [23] are indicated by open squares. HFBLN results are drawn as a solid curve.

Figure 10: Neutron quasiparticle routhians as function of the angular velocity for the ground SD band of the nucleus ^{190}Hg. The convention for the different (parity, signature) combinations is: $(+,+)$ solid line, $(+,-)$ dashed line, $(-,+)$ dot-dashed line, $(-,-)$ dotted line.

Figure 11: Same as in Fig. 10 for protons in ^{192}Hg

Figure 12: Same as in Fig. 10 for ^{192}Hg.

Figure 13: Comparison of the evolution of selected neutron quasiparticle routhians as function of the angular velocity for the ground SD bands of the nuclei ^{190}Hg, ^{192}Hg, ^{193}Hg (see text) and ^{194}Hg. The convention for the different (parity, signature) combinations is the same as in Fig. 10.

Figure 14: Same as in Fig. 10 for ^{194}Pb.