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## Superdeformed single-particle orbitals in the $A = 190$ region from Hartree-Fock plus BCS calculations

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Self-consistent axial Hartree-Fock plus BCS calculations have been performed in order to analyze the superdeformed single-particle orbitals near the chemical potentials in Hg and Pb nuclei. The influence of an approximate restoration of the particle-number symmetry is investigated. A discussion of available data is made, taking stock of our results, in the framework of the strong coupling model.

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### I. INTRODUCTION

Prompted by recent microscopic calculations [1–3] many experimental groups [4–23] have identified more than 25 superdeformed (SD) bands at rather low spins (indeed as low as about  $8\hbar$ ) in the  $A = 190$  region. The evidence of a secondary minimum, however, had been previously suggested by theoretical results obtained in this region, both in Hartree-Fock plus BCS calculations [24] and in Strutinsky-type calculations [25–28]. Indeed no special attention to the consequences on coexisting largely deformed states had been paid then. In Ref. [1], the existence of SD states at low spin has been specifically predicted from the results of extensive lattice Hartree-Fock calculations. In these static calculations, local equilibrium deformations have been found to be stable against both triaxial and parity breaking modes. In the latter case, however (odd multipolarity modes), a significant softness has been recently advocated in some nuclei from both experimental [11] and theoretical [29,30] studies. It is to be noted that, contrarily to what appeared to be the case in the  $A = 150$  region, the rotational lowering of the fission barrier is not necessary here to yield SD pockets, even though finite angular velocities are effective in stabilizing such SD states at higher spins [3,28,31].

The importance of pairing correlations is quite obvious for a correct description of deformation (static and all the more dynamical) properties. In any situation where the chemical potential is close to a magic number it is rather crucial to go beyond the current BCS approximation which is known to be defective in the weak pairing limit. Recently [32], an approximate restoration of the particle-number symmetry has been explicitly incorporated in our Hartree-Fock plus BCS approach within the Lipkin-Nogami (LN) framework [33]. It will, as a general rule, effectively increase pairing gaps in the considered limit with obvious consequences on quasiparticle energies. Such effects have been recently investigated in

rare-earth nuclei by Nazarewicz *et al.* [34]. The aim of the present work is to perform a similar study for SD states in odd Hg and Pb isotopes. In doing so we are taking stock of the good reproduction [35] of the spectroscopic properties in  $^{237}\text{Pu}$  and  $^{239}\text{Pu}$  fission isomers [36] which was the first available source of such data. A preliminary account of this study has been already reported in Ref. [37].

We will analyze here single-particle neutron and proton orbitals near the chemical potentials extracted from our microscopic calculations in order to (i) predict the location and nature of rotational bandheads, (ii) illustrate the influence of a correct treatment of pairing correlations on the former, and (iii) compare for some isotopes, such as  $^{193}\text{Hg}$ ,  $^{194}\text{Hg}$ ,  $^{194}\text{Tl}$ , the experimental data with the results of a simple rotor plus quasiparticle approach stemming from our microscopic results.

### II. THE SINGLE-PARTICLE SPECTRA

Hartree-Fock plus BCS calculations have been performed assuming axial symmetry and upon projecting single-particle wave functions on axially deformed harmonic-oscillator states according to the method developed in Ref. [38]. The basis size is equivalent to 13 major shells and a proper optimization of the two oscillator frequencies has been performed. The nucleon-nucleon force in use is the Skyrme III effective interaction [39] which has proven (see, e.g., in a similar physical situation [35]) to yield very good single-particle properties. Another parametrization, known as the SkM\* force [40] (used also, e.g., in the SD calculations of Ref. [1]), has not the same spectroscopic quality but leads to better bulk properties at large deformations due to its correct surface tension (which happens to be lower than the one obtained with the Skyrme III force). This has the consequence, for instance, to lead to a slight underestimation of the quadrupole moments of SD solutions calculated

TABLE I. Comparison of calculated and experimental quadrupole ( $Q_2$ ) and hexadecapole ( $Q_4$ ) moments for the mass and charge (ch) distributions. The  $Q_2$  ( $Q_4$ ) moment values are given in  $e^2 b$  ( $e^4 b^2$ ).

Nucleus		$^{190}\text{Hg}$	$^{192}\text{Hg}$	$^{194}\text{Hg}$	$^{192}\text{Pb}$	$^{194}\text{Pb}$	$^{196}\text{Pb}$	$^{198}\text{Pb}$	$^{200}\text{Pb}$
HF+BCS	$Q_2^{\text{mass}}$	42.1	42.7	44.0	42.7	44.8	45.0	44.4	44.5
	$Q_2^{\text{ch}}$	18.1	18.2	18.5	18.7	19.3	19.2	18.8	18.7
	$Q_4^{\text{ch}}$	4.06	4.09	4.05	4.20	4.4	4.25	4.0	3.9
Strutinsky Ref. [41]	$Q_2^{\text{ch}}$			18.8					
	$Q_4^{\text{ch}}$			3.9					
Experiment [Refs. 9 and 10]	$Q_2^{\text{ch}}$	19±3	20±2						

with the Skyrme III.

The multipole moments which are not trivially vanishing due to the retained symmetries are not free parameters but self-consistently determined from our local equilibrium static solutions. The calculated mass and charge quadrupole moments  $Q_2$  and the charge, hexadecapole moments  $Q_4$  of  $^{190,192,194}\text{Hg}$  and  $^{192,194,196,198,200}\text{Pb}$  are listed in Table I. They are compared with the results of the Strutinsky approach calculations of Ref. [7] for  $^{194}\text{Hg}$ , upon converting the deformation parameters  $\beta_2=0.465$ ,  $\beta_4=0.055$  into multipole moments according to the approximate formulas of Ref. [41] with a

standard-size parameter value ( $r_0=1.27$  fm for protons). As seen in Table I both calculations agree for the charge moments  $Q_2$  and  $Q_4$  of superdeformed states. Our results fall also very well into experimental error bars [9,10] as far as charge  $Q_2$  moments are concerned for  $^{190}\text{Hg}$  and  $^{192}\text{Hg}$ .

At these deformations determined for each considered nucleus, one gets single-particle neutron (proton) spectra displayed in Fig. 1 (Fig. 2). The isotropic and isotonic differences are indeed rather weak apart from well-understood translations when varying one nucleon number, keeping the other fixed. The  $^{194}\text{Hg}$  spectra of Ref.

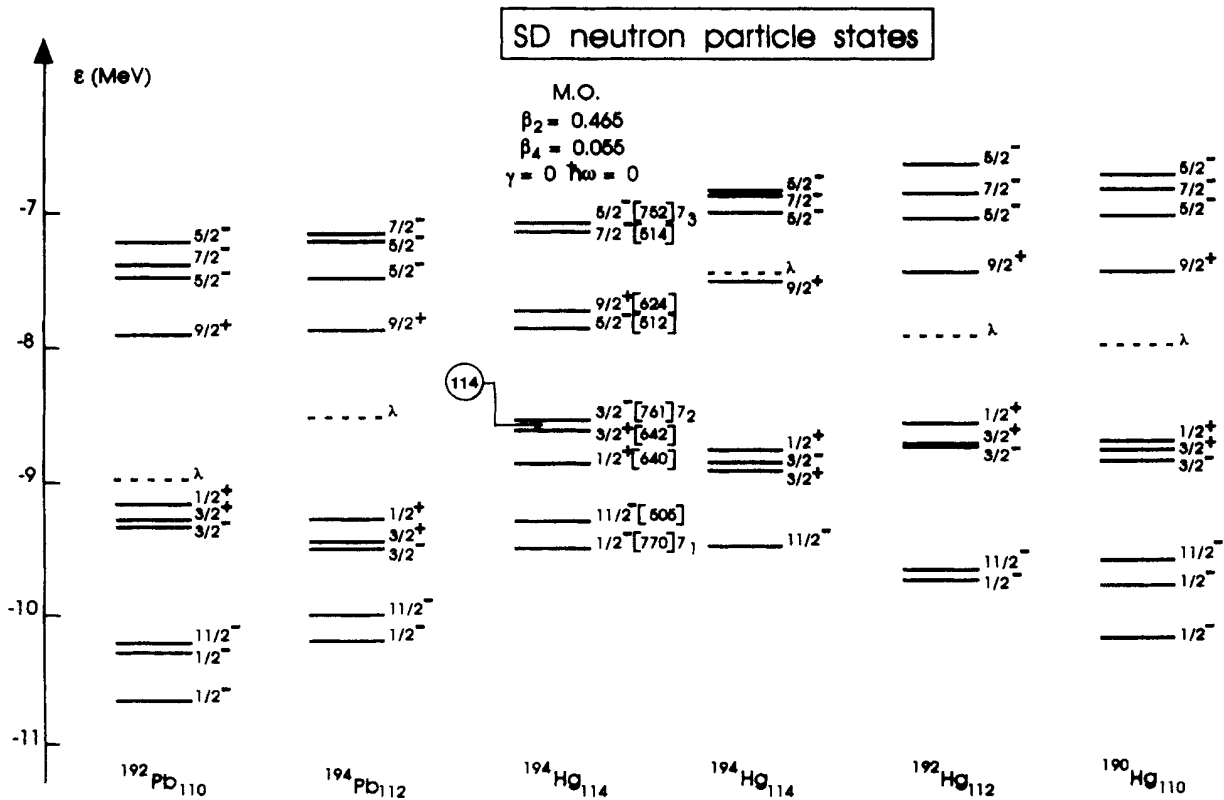


FIG. 1. Single-particle neutron spectra obtained in constrained Hartree-Fock plus BCS calculations at the superdeformed minimum for  $^{190,192,194}\text{Hg}$  and  $^{192,194}\text{Pb}$ . The spectrum obtained in cranked shell model using a modified oscillator (M.O.) is also displayed for  $^{194}\text{Hg}$ . In the microscopic calculations, the chemical potential ( $\lambda$ ) energy is shown as a dashed line.

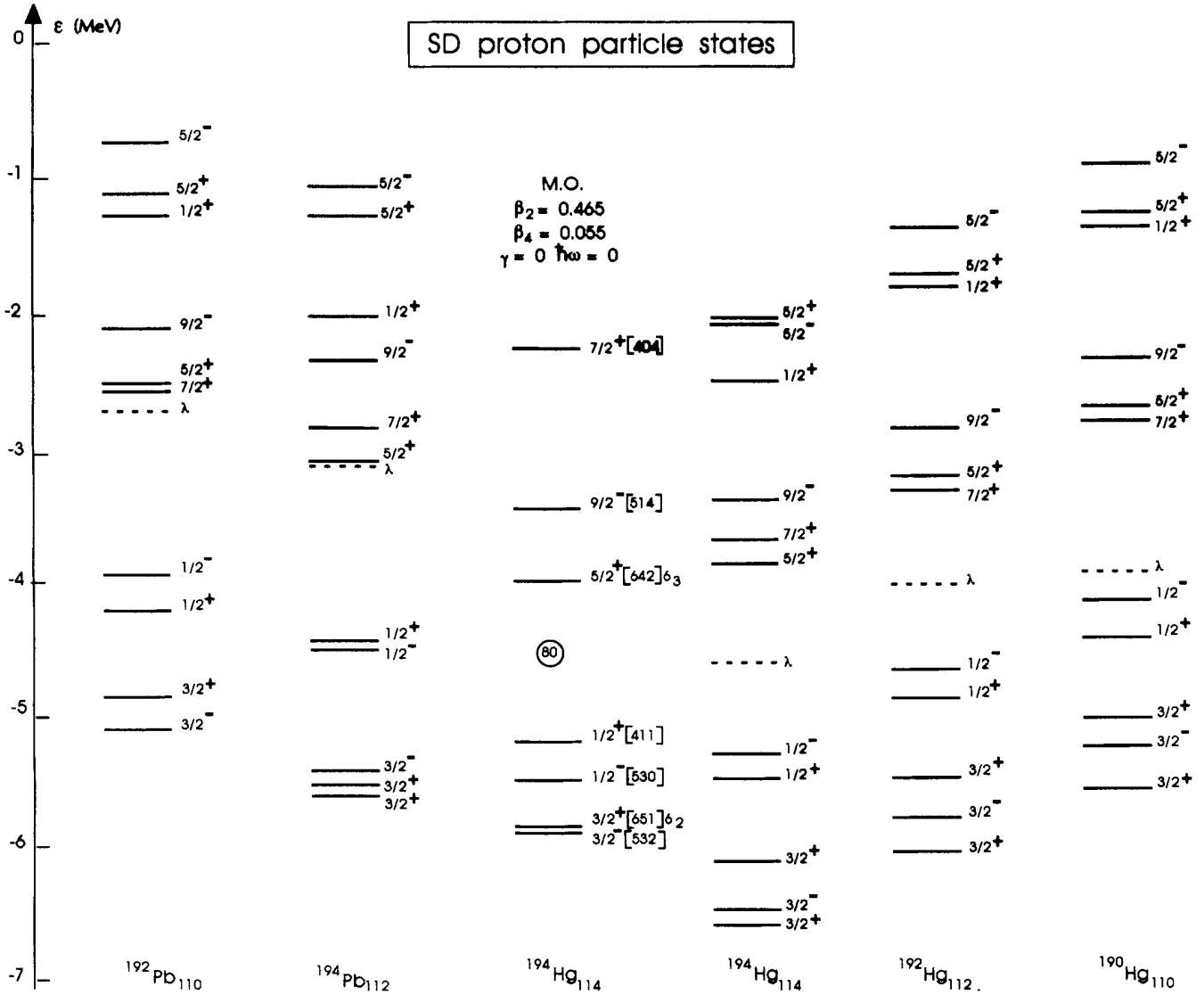


FIG. 2. Same as Fig. 1 for protons.

TABLE II. Main components of the superdeformed single neutron states located near the Fermi level in the  $^{194}\text{Pb}$  nucleus obtained in Hartree-Fock + BCS calculations using the SIII effective force. Under the label  $[Nn_z\Lambda]$  are displayed the sum of various contributions corresponding to the same values of  $\Lambda$  and different values of  $N$  and  $n_z$ .

$\frac{7}{2}^-$	[514]		69%[514]	17%[714]	6%[734]	2%[523]			
			86%						
$\frac{5}{2}^-$	[752]	$7_3$	24%[752]	9%[532]	6%[732]	23%[972]	3%[1192]	14%[712]	7%[ $Nn_z3$ ]
$\frac{5}{2}^-$	[512]		24%[512]	20%[312]	21%[712]	2%[912]	20%[732]	2%[752]	2%[972]
			67%						
$\frac{9}{2}^+$	[624]		58%[624]	17%[824]	13%[844]	2%[1044]	2%[604]	3%[ $Nn_z5$ ]	
			75%		15%				
$\frac{1}{2}^+$	[640]		18%[640]	9%[440]	3%[840]	20%[860]	9%[620]	4%[420]	3%[820]
			30%			16%			
			7%[431]	3%[871]	7%[ $Nn_z1$ ]				

TABLE III. Same as Table II for protons.

$\frac{7}{2}^+$	[404]	67%[404]	25%[804]	3%[604]	2%[624]				
		95%							
$\frac{9}{2}^-$	[514]	59%[514]	25%[714]	2%[914]	9%[734]	2%[934]			
		86%			11%				
$\frac{5}{2}^+$	[642]	6 <sub>3</sub>	26%[642]	3%[842]	9%[422]	11%[622]	3%[822]	26%[862]	5%[1082]
			29%		23%				
$\frac{1}{2}^+$	[411]	28%[411]	22%[211]	25%[611]	4%[811]	9%[631]	3%[831]	3%[ $Nn_20$ ]	
			79%			12%			
$\frac{1}{2}^-$	[530]	19%[530]	7%[330]	14%[330]	20%[750]	4%[950]	6%[970]	7%[ $Nn_21$ ]	
			40%		24%				
		7%[510]	3%[710]	4%[110]	2%[310]				
			16%						

[7] are also displayed. They compare reasonably well with what we have obtained for this isotope. In particular any given orbital is found in both calculations at about the same energies (within some hundred keV with very few exceptions as the  $[404] \frac{7}{2}^+$  proton and  $[512] \frac{5}{2}^-$  neutron states).

It is worth analyzing in detail the structure of some of these single-particle wave functions. As it is usual, the asymptotic quantum number labeling is quite inadequate as shown in Tables II and III for the levels closed to the chemical potential. For instance, in  $^{194}\text{Pb}$  the so-called  $[640] \frac{1}{2}^+$  neutron state has only a 18% probability of being in that basis state and a similar result holds for the  $[530] \frac{1}{2}^-$  proton state (19%). More interesting in some instances, decoupling parameters, magnetic properties, etc., would be a detailed analysis of the spin content of such states.

### III. EFFECT OF THE LIPKIN-NOGAMI APPROXIMATE SYMMETRY RESTORATION

In Ref. [32], where a summary of the formalism and some computational details are given, the consequence of the LN pairing treatment for potential energy surfaces was discussed. This was exemplified there in particular for the SD well of  $^{196}\text{Pt}$ . Indeed the second well excitation energy and the inner barrier height were found to exhibit only slight modifications for this isotope (respectively, changing by 0.2 and 0.25 MeV). As a matter of fact, such a conclusion is to be generalized in all cases where, at the deformations under consideration, the level density is large enough so that one is not in the weak pairing limit.

As already mentioned, the effect of the LN treatment on quasiparticle energies has been studied in the rare-earth region by Nazarewicz, Riley, and Garrett [34]. A possible approximate description of the energy of odd-even nuclei would consist in a Lipkin-Nogami approach

with blocking. Indeed by blocking one single-particle Hartree-Fock level (generally for any practical use near the chemical potential) one substantially decreases the effective level density, making it very important to ade-

SD neutron quasiparticle states

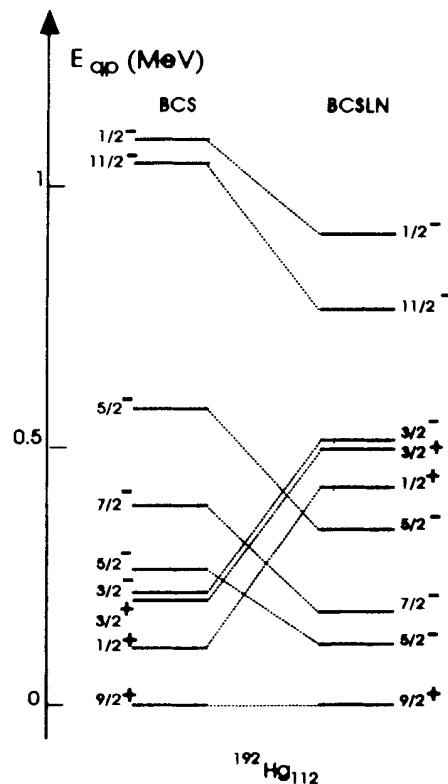


FIG. 3. Comparison of superdeformed single quasiparticle neutron spectra obtained in the usual BCS approximation (BCS) and in the Lipkin-Nogami treatment (BCSLN) for  $^{192}\text{Hg}$ .

SD proton quasiparticle states

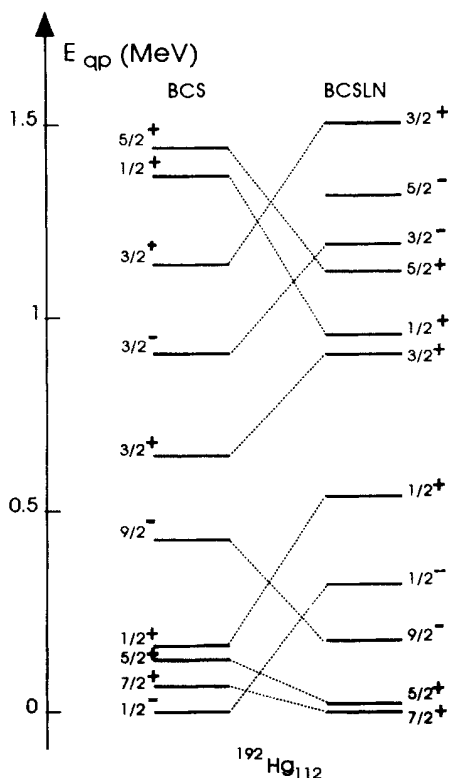
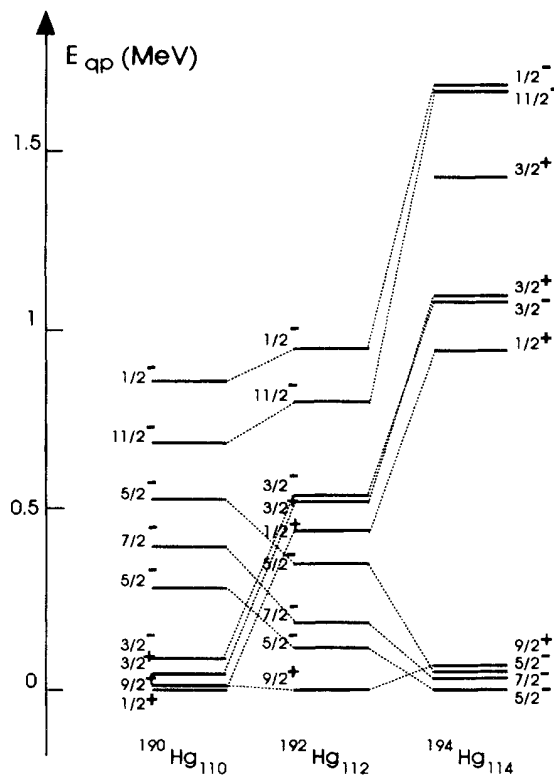


FIG. 4. Same as Fig. 3 for protons.

quately describe the pairing correlations in this limit (see, e.g., Ref. [42]). The use of the wave functions resulting from a LN treatment would as a matter of fact be affected by two difficulties: (i) *a priori* such an approximate LN method does not lead to wave functions of any relevance, being an approximate variational approach merely for the energy observable; (ii) even though one would take it as an approximate ansatz for that matter, one would have to face difficult problems of orthonormalization when using more than one configuration with the same quantum numbers. In view of the present study including a rotor plus quasiparticle approach which will be discussed below, we found that a satisfactory compromise could consist in considering one quasiparticle states out of a quasiparticle vacuum treated in the manner of Lipkin-Nogami.

As a result, illustrated on Figs. 3 and 4, for the neutron and proton spectra in  $^{192}\text{Hg}$ , one sees clearly that a more correct pairing treatment yields differences in free quasiparticle energies (with respect to a standard BCS treatment) typically of about 200–300 keV. The level ordering is also affected accordingly. The variations of the neutron (proton) free quasiparticle energies, within the Lipkin-Nogami treatment, are displayed on Figs. 5 and 6 (Figs. 7 and 8) for Hg and Pb isotopes. For each different isotope, the core deformation has resulted from fully self-consistent calculations as described above. This is of relevance since their energies are in some cases varying

SD neutron quasiparticle states

FIG. 5. Variations of the superdeformed quasiparticle neutron spectra (with the Lipkin-Nogami treatment) for the  $^{190,192,194}\text{Hg}$  isotopes.

very much with the deformation. However, one should note that the price to pay for the simplicity (orthogonality of the states) of our approach is the absence of any polarization effects. In that respect one must distinguish between such effects at the same deformation which are out of reach for Strutinsky-type calculations as those of Ref. [34] as opposed to the polarization effect of deformation-driving orbitals which could be included in such approaches. Of course, potentially, we should be able to yield both effects in our approach. It would remain, however, difficult to treat correctly the spin-polarization effects since within the Skyrme-Hartree-Fock formalism, for nontime-reversal-invariant solutions one should then consider a substantial amount of supplementary densities [43].

#### IV. DISCUSSION

A direct comparison of the quasiparticle energies (as those of Figs. 5, 6, 7, and 8) with experimental band head energies is only possible if one can rule out any coupling with collective modes. As far as the rotational mode is concerned we have addressed this question within the microscopic rotor plus one quasiparticle approach of Refs. [44 and 45]. In the odd mercury isotopes, for instance (as in most nuclei under consideration here) there are very

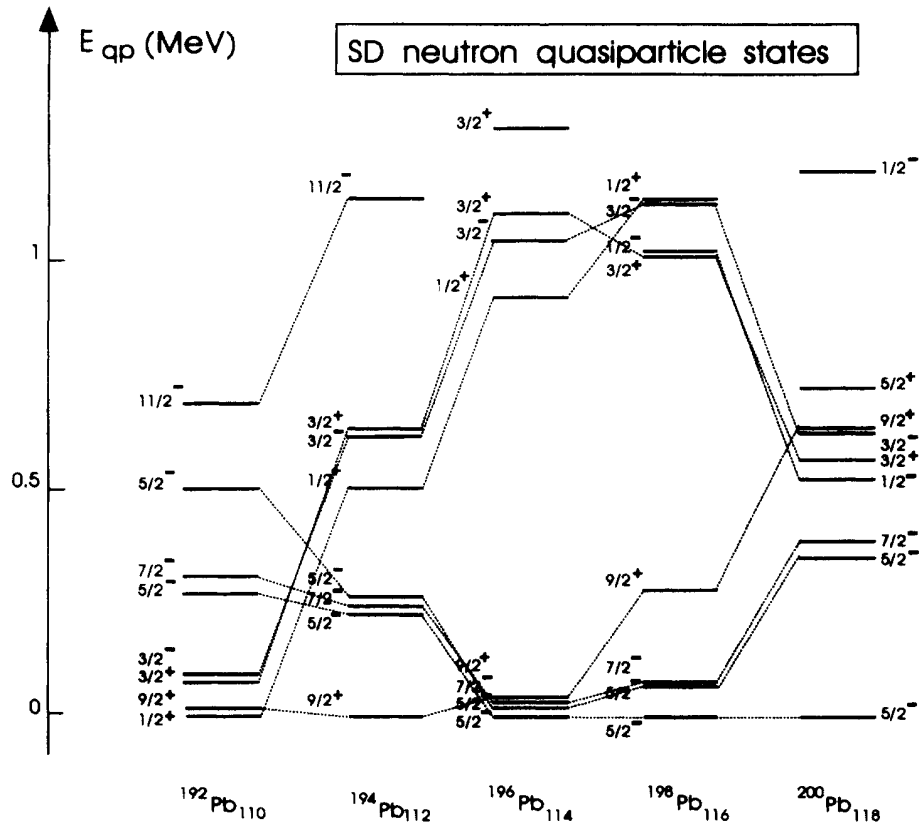


FIG. 6. Variations of the superdeformed quasiparticle neutron spectra (with the Lipkin-Nogami treatment) for the  $^{192,194,196,198,200}\text{Pb}$  nuclei.

few cases in which states able to be coupled would lie sufficiently close in energy. This fact supplemented by the large value of the moment of inertia explains why, upon diagonalizing the rotor plus one quasiparticle Hamiltonian, we have indeed found that, in most cases, it is safe to consider this coupling as ineffective. The only clean-cut exception to that, concerns the neutron bands labeled  $[512] \frac{5}{2}^-$  and  $[514] \frac{7}{2}^-$  which lie, before coupling, within less than 100 keV in the  $^{194}\text{Hg}$  isotope, for instance.

In the framework of one or two quasiparticles plus rotor model we will now comment on the band structure of odd, even-even, and odd-odd SD states of Hg, Tl, and Pb isotopes. In  $^{193}\text{Hg}$ , four bands have been clearly identified by Cullen *et al.* [11] with lowest spin states being estimated, respectively, as being  $\frac{15}{2}$ ,  $\frac{21}{2}$ ,  $\frac{19}{2}$ , and  $\frac{27}{2}$ . Upon coupling one neutron quasiparticle to the  $^{192}\text{Hg}$  (or  $^{194}\text{Hg}$ ) core, one predicts four bandheads in less than 350 keV (or 100 keV), concerning, namely, the orbitals labeled as  $[624] \frac{9}{2}^+$ ,  $[512] \frac{5}{2}^-$ ,  $[514] \frac{7}{2}^-$ , and  $[752] \frac{5}{2}^-$ . For each bandhead one expects in the strong coupling limit two cascades of  $E2$  transitions ( $I+4 \rightarrow I+2 \rightarrow I \dots$ ) and ( $I+5 \rightarrow I+3 \rightarrow I+1 \dots$ ), i.e., resulting thus into the appearance of eight SD band structures. The assignment of the four observed SD bands in terms of signature ( $\alpha$ ) partners [11]  $[512] \frac{5}{2}^- \alpha = -\frac{1}{2}$  for band 1,  $[512]$

$\frac{5}{2}^- \alpha = +\frac{1}{2}$  or  $[624] \frac{9}{2}^+ \alpha = +\frac{1}{2}$  for band 2,  $[624] \frac{9}{2}^+ \alpha = -\frac{1}{2}$  for band 3, and  $[752] \frac{5}{2}^- \alpha = -\frac{1}{2}$  for band 4 are partly confirmed by our microscopic calculations. However, the vicinity in energy of the four neutron quasiparticle states does suggest that four supplementary SD bands should be present in the  $^{193}\text{Hg}$  isotope.

As for the  $^{191}\text{Hg}$ , the  $[624] \frac{9}{2}^+$ ,  $[640] \frac{1}{2}^+$ ,  $[642] \frac{3}{2}^+$ ,  $[761] \frac{3}{2}^-$ , and  $[512] \frac{5}{2}^-$  quasineutron states are calculated here very close in energy (less than 300 keV for the  $^{190}\text{Hg}$  core). This makes it very difficult to conclude on the assignment of the single band which has been observed so far [4].

Within our approximate approach, the description of the odd proton  $^{193}\text{Tl}$  nucleus can be made *a priori* in terms of either one quasiproton plus a  $^{192}\text{Hg}$  core or one quasiproton plus a  $^{194}\text{Pb}$  core. In both cases the lowest quasiparticle orbitals involved are found to be the  $[404] \frac{7}{2}^+$ ,  $[642] \frac{5}{2}^+$ , and  $[514] \frac{9}{2}^-$  states; we partly confirm the assignment  $[642] \frac{5}{2}^+$  given for the two observed SD bands in Ref. [13] but we cannot completely rule out the two other possibilities.

The strong coupling of two valence quasiparticle of neutron would give rise in  $^{194}\text{Hg}$  to multiple SD cascades, as the four observed experimentally in Ref. [7]. Selecting only, for the  $^{192}\text{Hg}$  core, the high- $K$  configuration bandheads value such as

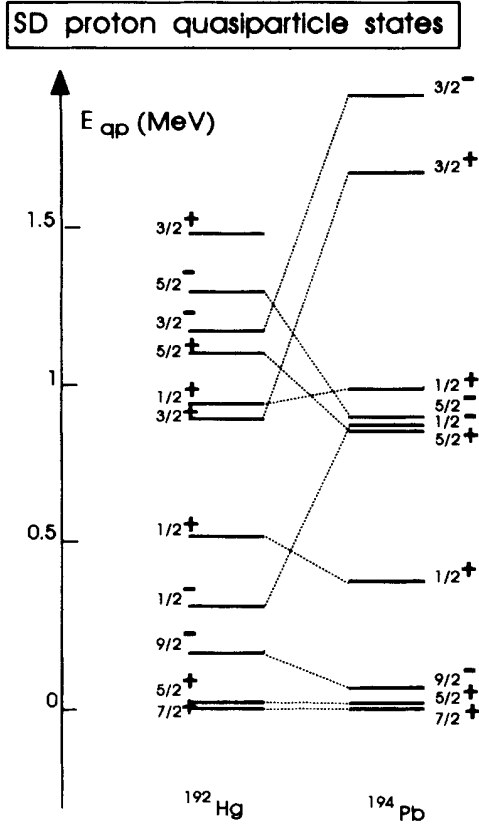


FIG. 7. Variations of the superdeformed quasiparticle proton spectra (with the Lipkin-Nogami treatment) for the  $^{192}\text{Hg}$  and  $^{194}\text{Pb}$  nuclei.

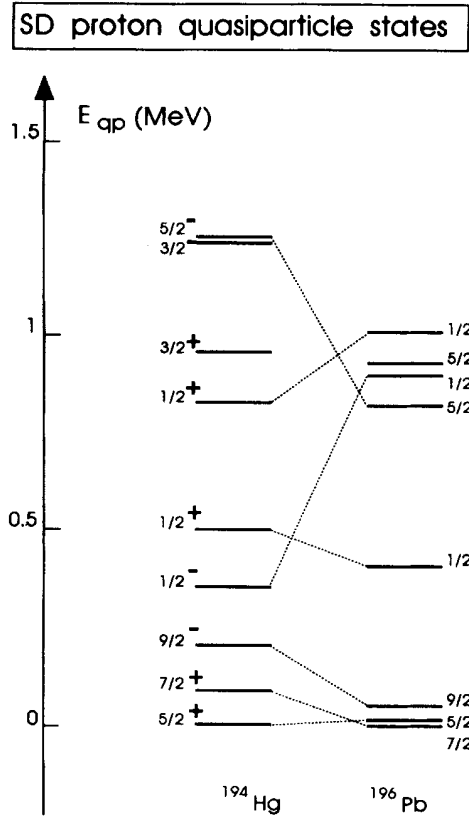


FIG. 8. Variations of the superdeformed quasiparticle proton spectra (with the Lipkin-Nogami treatment) for the  $^{194}\text{Hg}$  and  $^{196}\text{Pb}$  nuclei.

$$\begin{aligned}
 & ([624] \frac{9}{2})^2 K^\pi = 8^+ (0), \\
 & ([624] \frac{9}{2} * [512] \frac{5}{2}) K^\pi = 7^- (0.132), \\
 & ([624] \frac{9}{2} * [514] \frac{7}{2}) K^\pi = 8^- (0.196), \\
 & ([512] \frac{5}{2} * [514] \frac{7}{2}) K^\pi = 6^+ (0.328), \\
 & ([624] \frac{9}{2} * [752] \frac{5}{2}) K^\pi = 7^- (0.396), \\
 & ([512] \frac{5}{2} * [752] \frac{5}{2}) K^\pi = 5^+ (0.528),
 \end{aligned}$$

etc., where the values in parentheses are energies relative to the lowest configuration ( $K^\pi = 8^+$ ) expressed in MeV, several bands can be predicted. It is clear, however, that the preceding corresponds to a very crude strong coupling approximation. In particular, it obviously neglects interaction effects between the last two neutrons.

The  $^{194}\text{Pb}$  SD band has been identified and described by Theine *et al.* [17] in terms of two protons in the  $[642] \frac{5}{2}^+$  and  $[514] \frac{9}{2}^-$  orbitals above  $^{192}\text{Hg}$  core. Our calculations show that the  $[404] \frac{7}{2}^+$  orbital could also play a role in this nucleus and that several SD bands could as well exist.

The same can be argued for the odd-odd  $^{194}\text{Tl}$  isotope where Azaiez *et al.* [14,15] have identified six SD bands grouped in three sequences. Our microscopic valence quasiparticle SD states for neutrons and protons are the following (see Figs. 6 and 7):  $[512] \frac{5}{2}^-$ ,  $[624] \frac{9}{2}^+$ ,  $[524] \frac{7}{2}^-$ ,  $[752] \frac{5}{2}^-$  for neutrons and  $[404] \frac{7}{2}^+$ ,  $[642] \frac{5}{2}^+$ ,  $[514]$

$\frac{9}{2}^-$  for protons. Therefore 12 candidates for SD bandheads, in less than 500 keV, should *a priori* emerge from the high- $K$  values odd-odd configurations; however, if we take crudely into account the residual proton-neutron interaction between the two free quasiparticles with the simplistic<sup>1</sup> Gallagher-Moskowski rule [46], the lowest SD bandheads would be

$$\begin{aligned}
 & (\pi[642] \frac{5}{2}^+ * \nu[624] \frac{9}{2}^+) K^\pi = 7^+ (0), \\
 & (\pi[642] \frac{5}{2}^+ * \nu[512] \frac{5}{2}^-) K^\pi = 5^- (0.132), \\
 & (\pi[514] \frac{9}{2}^- * \nu[624] \frac{9}{2}^+) K^\pi = 9^- (0.150), \\
 & (\pi[404] \frac{7}{2}^+ * \nu[514] \frac{7}{2}^-) K^\pi = 7^- (0.181), \\
 & (\pi[514] \frac{9}{2}^- * \nu[512] \frac{5}{2}^-) K^\pi = 7^+ (0.282), \\
 & (\pi[624] \frac{5}{2}^+ * \nu[752] \frac{5}{2}^-) K^\pi = 5^- (0.396), \\
 & (\pi[514] \frac{9}{2}^- * \nu[752] \frac{5}{2}^-) K^\pi = 7^+ (0.546),
 \end{aligned}$$

<sup>1</sup>“Simplistic” should be understood here in two ways. First it is, after all, merely an empirical rule. More importantly, its use here makes the highly crude assumption that a state labeled  $[404] \frac{7}{2}^+$ , for instance, is an eigenstate of the spin projection operator corresponding to a spin-down state. This, as recalled in Sec. II, overlooks the possibility of a spin mixing due to the self-consistent mean field.



where, as in the previous discussion of  $^{194}\text{Hg}$ , the values in parentheses (expressed in MeV) correspond to the energies of free neutron and proton quasiparticles. One knows from the study of Ref. [47], that taking into account in a consistent fashion the residual interaction can change the bandhead energies by a few hundred keV. Nevertheless, it is plausible that several SD cascades should be present at low energy in this nucleus beyond the six presently observed. They might, however, correspond to a very weak part of the intensity due to the sharing of a global probability which is weak anyway.

Finally, we are able to predict and assign SD bands from the Fig. 6 for odd lead nuclei where SD bands remain yet unobserved.

## V. CONCLUSIONS

In this paper we have demonstrated that a correct treatment of the pairing correlations is of prominent importance to properly describe superdeformed bandheads in the  $A=190$  mass region. Microscopic rotor plus quasiparticle calculations have confirmed that Coriolis interaction effects are negligible in most cases. However, due to the rather high single-particle densities in this region, a more consistent treatment of the interaction of valence quasiparticles between themselves and with the

core, remains in some cases to be performed. The latter could show up to be very instrumental for an accurate assignment of the lowest superdeformed bandheads.

We have predicted that some superdeformed bands, other than those already observed, could be experimentally identified in these nuclei. For this, sophisticated gamma multidetector arrays such as EURO-GAM or GAM-MASPHERE appear to be an absolute necessity.

*Note added*—While preparing this paper, a paper by W. Satula, S. Cwiok, W. Nazarewicz, R. Wyss, and A. Johnson [Nucl. Phys. **A529**, 289 (1991)] dealing with a similar subject, came to our knowledge. Qualitatively we agree with their bandhead findings.

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