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Hartree-Fock-Bogoliubov calculations of the rotational band of the very heavy ^{254}No nucleus

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This paper is dedicated to the memory of Jordanka Piperova

Abstract. We report on Hartree-Fock-Bogoliubov (HFB) calculations of the ground-state rotational band of the heavy nucleus ^{254}No recently observed experimentally. The calculated quadrupole deformation is consistent with the experimental value of $\beta = 0.27$ and is almost constant over the whole band. We also reproduce fairly well the excitation spectra and moments of inertia of this isotope up to the maximal experimentally observed state of spin 20. The rather high stability of this nucleus against fission is illustrated by the deformation energy curve providing very high fission barriers at zero spin within the HFB and HFB plus Lipkin-Nogami formalisms. The variation of these barriers with increased angular velocities is also studied.

PACS. 21.10.Re Collective levels – 21.60.Ev Collective models – 21.60.Jz Hartree-Fock and random-phase approximations

After the Cohen, Plasil and Swiatecki [1] seminal study of the stability of rotating liquid drops, very heavy nuclei with mass greater than 250 are generally expected to survive rotational excitation only up to rather low spins. Of course, large shell correction energies added to the bulk liquid drop estimates may lead to sizable enhancements of the stability against fission in some cases. Observation of relatively high-spin states in very heavy nuclei thus provides a very useful tool to assess any theoretical description of shell effects in this mass region, which is of primary importance for a good prediction of shell-stabilized superheavy elements.

The experimental observation in the ground-state band of the ^{254}No nucleus of rotational states from spins 4 to 18 $\hbar$ (and tentatively 20 $\hbar$) has been reported recently in a series of papers [2–4]. These experiments have been performed using ^{48}Ca beams from 130 to 219 MeV on ^{208}Pb targets. Two of them (including the more recent) were conducted at the Argonne National Laboratory with the Gammasphere 4π Ge detector array, while the other made use of four Ge clover detectors and was performed at the University of Jyväskylä. In all three experiments, the ^{254}No nuclei were implanted into a position-sensitive Si strip detector placed at the focal plane. The γ-rays coming from the ^{254}No were unambiguously identified from the coincidence with the α-decay chain in the Si detector. As the transition to the ground state have not been observed, the spin assignment relies on the use of a Harris parameterization for both $J^{(1)}$ and $J^{(2)}$ moments of inertia.

In ref. [4], the authors proposed a new method to deduce the fission barrier height $B_{\rm f}$ based on a reconstruction of the entry distribution of the evaporation residues in spin and excitation energy. Since the fission process above the saddle-point energy should be much favored compared to the γ-emission, they claim that for any given observed spin, the maximal excitation energy of the entry distribution should lie below the saddle-point energy. For each spin the end-point of the excitation energy distribution gives thus a lower bound for the fission barrier height which is estimated to be greater than 5 MeV around $I = 12\ \hbar$.

In a recent paper involving some of the authors [5], it has been shown using state-of-the-art semiclassical calculations, namely in the extended Thomas-Fermi (ETF) approach, that the rotating liquid drop model had to be refined by including a spin dependence of its parameters

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which, as a result, provides a fission stability of heavy nuclei upon increasing the spin, which is enhanced with respect to what is stated in ref. [1]. It is the aim of the present paper to go beyond this work, describing altogether bulk properties as well as shell and pairing effects within the fully self-consistent microscopic Hartree-Fock-Bogoliubov (HFB) formalism, in the particular case of ^{254}No.

In our calculations, we have used the triaxial Hartree-Fock-Bogoliubov code developed by Laftchiev *et al.* [6,7]. This code is an extension of the Hartree-Fock Routhian code presented in refs. [8,9] which uses Skyrme-type effective interactions and assumes parity and signature as symmetry operators for the one-body Hamiltonian. There, solutions breaking time-reversal symmetry are described through a decomposition of the single-particle wave functions on an axially symmetric harmonic-oscillator basis. The triaxial character inherent to the solutions of this formalism is taken care of by a decomposition of the various densities as Fourier series in the azimuthal angle. This particular choice provides shorter computation times than usual triaxial codes as for instance those of refs. [10, 11]. The pairing correlations are described à la HFB with particle number projection tentatively taken into account within the approximate Lipkin-Nogami (LN) scheme [12, 13]. The latter method which is widely used for instance in the context of fully self-consistent microscopic calculations (see *e.g.*, ref. [14] for time-reversal symmetric Hamiltonians, or ref. [15] for Routhian calculations) results in the addition of a constraint on the second-order fluctuations of the particle number. However it has been shown [16] in the $A \simeq 190$ mass region from calculations using the Gogny force that this approximation could produce somewhat inconsistent results.

The HFB equations may be cast into a usual eigenvalue form in a doubled space where the 2×2 "Hamiltonian" is defined in terms of the Hartree-Fock Hamiltonian h and of the pairing potential Δ, whereas the eigensolutions are the usual U and V matrices (see for the notations, *e.g.*, [17]). Similarly to what was done in ref. [15], these equations are solved in two steps at each iteration. First we solve simple Hartree-Fock equations (that is the HFB equations with vanishing pairing field) to obtain the eigenstates of the Hartree-Fock–like Hamiltonian. Then the original equations are solved in a truncated configuration space (through an energy cutoff) of the Hamiltonian eigenstates previously determined.

For the particle-hole channel, we have used the SkM* parameterization of the Skyrme interaction [18] since it was originally fitted to provide a good description of the ^{240}Pu fission barrier and is thus rather well adapted to describe the stability against fission in very heavy nuclei. In the particle-particle channel, we have simply used the "modified seniority pairing force" previously described by Gall *et al.* in ref. [15]. At the present stage of our investigations of rotational properties in very heavy nuclei, we have not attempted to make a global fit over a variety of different nuclei to provide a pairing force which could be deemed to be somewhat universal in this mass region. We rather satisfied ourselves with a parameterization yielding the right moment of inertia at very low spins to assess the validity of our approach in reproducing the transition energies and moment of inertia (at higher spins). The matrix elements $G_{\rm n}$ and $G_{\rm p}$ for neutrons and protons are defined with the usual prescription $G_q = g_q/(11 + N_q)$, N_q being the number of particles in the charge state q. The value of $g_{\rm n}$ ($g_{\rm p}$, respectively) is 14.3 MeV (15.5 MeV, respectively) in the pure HFB case and 10.65 MeV (14.1 MeV, respectively) in the HFB + LN case with an energy cutoff 6.2 MeV above the Fermi level in both cases. No smeared boundary conditions for this configuration space have been taken into account yet which may locally create some minor technical deficiencies.

The calculations have been performed using the usual deformation-dependent truncation scheme equivalent to a 13 major shells spherical basis, corresponding to more than 450 harmonic-oscillator states (for both signatures). The basis deformation parameters that have been used in our HFB calculations were obtained through a minimization of the energy calculated within an axially and time-reversal symmetric HF + BCS formalism. At zero angular velocity non-axially symmetrical solutions have been forcefully searched out (due to the symmetry properties of the interaction, one would never explore as well-known non-axial solutions starting from a first iteration axially symmetrical ansatz). At finite spins, the solutions explicitly break the axial symmetry. As a result however, the solutions are almost axially symmetric since the γ angle never exceeds 1° along the rotational band which allows us to only take into account the 5 lowest-order Fourier series in the densities decomposition (see ref. [8]).

Recently, T. Duguet *et al.* [19] have presented the results of HFB + LN calculations which could be considered to be in essence rather similar to ours with two practical differences which are however not very substantial provided that the technical work is performed adequately (i) solutions of the HFB equations are computed on a spatial grid, ii) a zero-range force is used in the particle-particle channel). However, they used for the particle-hole channel the SLy4 parameterization [20,21] which is known to give in average (*i.e.*, semiclassically) significantly too high fission barriers [22]. This may be considered as a drawback to study fission stability properties. Another series of calculations for the same nucleus has been published quite recently [23] making use of the D1S Gogny force parameterization [24] which is known to be well suited to study fission barriers. No corrections for the particle number symmetry violation, *e.g.*, of the Lipkin-Nogami type, have been taken into account.

Along the rotational band of ^{254}No, the mass quadrupole moment Q_0 varies very slightly between 32.9 and 32.7 barn in our calculations. This corresponds to a deformation parameter of $\beta = 0.27$ identical to the experimental value. It is to be noted that we are there in perfect agreement with the experimental results [2–4] as well as with the theoretical results of T. Duguet *et al.* [19] yielding $Q_{20} = 32.8$ barn. The calculations of Egido and

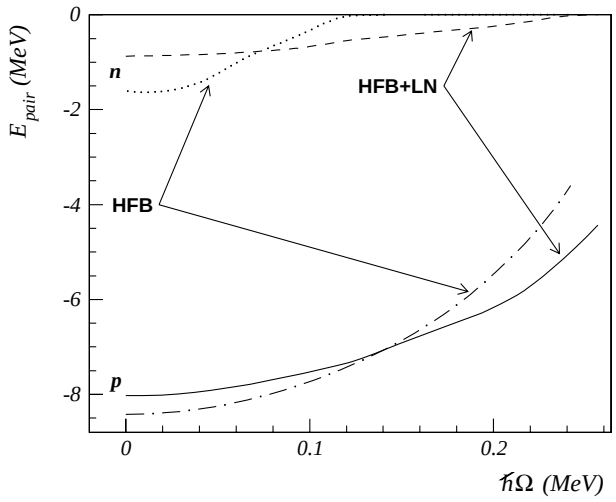

Fig. 1. Pairing energies (as defined in text) are plotted as functions of the angular velocity. Full and dashed lines (dash-dotted and dotted, respectively) correspond to proton and neutron energies calculated within the HFB + LN (pure HFB, respectively) formalism.

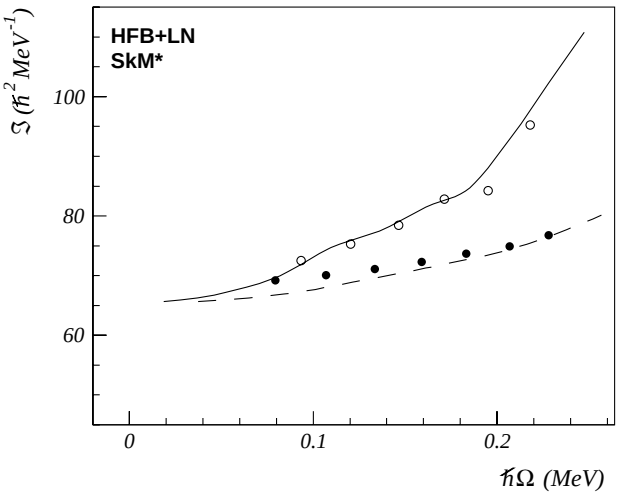

Fig. 2. Moments of inertia (see text) are plotted as functions of the angular velocity. Dynamic (kinematic, respectively) moment of inertia calculated within the HFB + LN formalism is displayed in full line (dashed, respectively) while its experimental counterpart is represented by open circles (full, respectively).

Robledo, on the other hand, yield slightly higher value of Q_{20}, resulting in a β-value close to 0.29.

We present in fig. 1 the evolution of the pairing energies, defined as a quantity proportional to the trace of the product of the abnormal density κ with the pairing potential Δ, for protons and neutrons with respect to the angular velocity Ω. It is well known from Nilsson-type calculations that for a deformation parameter of $\beta \simeq 0.3$ the $N = 152$ neutron number is magic [25]. This prediction is substantiated in our case by the rather low value of the neutron pairing energy compared to the proton corresponding energy. As usual in HFB calculations, the pairing energy is seen to decrease with increasing angular velocity. In particular, the neutron pairing energy vanishes above $\hbar\Omega = 0.22$ MeV. Within the same angular velocity range, the proton pairing energy is reduced by more than 40 percent.

It is clear from fig. 1, that around and above rotational frequencies of the order of $\hbar\Omega = 0.1$ MeV the results of pure HFB calculations are rather dubious as far as the neutron pairing correlations are concerned. This remark is clearly applicable also to the calculations of Egido and Robledo. It is generally expected that the Lipkin-Nogami corrected HFB calculations should be better adapted to such a situation of weak pairing correlations. However, as already mentioned, the calculations of Peru *et al.* (see, *e.g.*, [16]) in the superdeformed $A \simeq 190$ region show that the quality of the results of such an approach is rather unpredictable. The application to such a Routhian approach of pairing calculations conserving explicitly the particle number, *e.g.*, as those of Pillet *et al.* [26,27] would be of great interest there. In view of this expected inadequacy of pure HFB approach, we have therefore limited the discussion below of calculated moments of inertia to HFB + LN results.

The kinematic ($J^{(1)}$) and dynamic ($J^{(2)}$) moments of inertia are obtained from our calculations using the formulae

$$J^{(1)} = \frac{\langle \hat{j}_x \rangle}{\Omega} \tag{1}$$

$$J^{(2)} = \frac{\partial \langle \hat{j}_x \rangle}{\partial \Omega} \tag{2}$$

where $\hat{j}_x$ is the total angular momentum operator and Ω is the angular velocity. The derivative involved in the $J^{(2)}$ calculations have been taken over two consecutive even spins. Both are plotted in fig. 2 as functions of the angular velocity together with their experimental counterparts.

The kinematic moment of inertia $J^{(1)}$ is, in fact, the expression of the linear response of the system under the constraint of some collective variable. Nevertheless, we have actually assumed that it could be computed from the wave functions yielding the corrected energy (*i.e.*, bypassing an explicit treatment of LN corrections specific to $\langle j_x \rangle$ in the spirit of ref. [14]). It may also be argued that due to the dependence of λ_2 upon the angular velocity ω, eq. (2) is not correct and dynamic moments of inertia should be evaluated through second derivatives of the energy with respect to the spin. However, we have checked that this ω-dependence is very small and can be safely neglected (at least up to about $\omega = 0.1$ MeV).

It is seen in fig. 2 that we are reproducing rather well the experimental trend for both the $J^{(1)}$ and $J^{(2)}$ moments of inertia. The agreement of our results is better than the one obtained by Egido and Robledo for the only moment which they report, namely $J^{(1)}$. It is also better than the only moment reported by Duguet *et al.*, namely $J^{(2)}$ in this case. The latter is quite remarkable because, as it can be seen in fig. 3, our single-particle spectra are somewhat different for the neutron states. Whereas these authors find important deformed gaps feature around $N = 150$

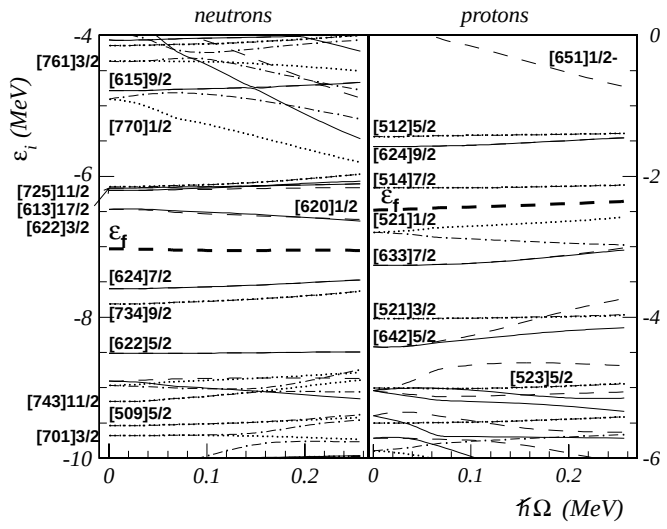

Fig. 3. Single-particle Routhians in the ^{254}No nuclei for neutrons (left panel) and protons (right panel) as a function of the angular velocity. The convention used for the (parity, signature) representation is the following: (+,+) in full lines, (+, −) in dashed lines, (−, +) in dash-dotted lines and (−, −) in dotted lines. Calculations are performed within the HFB + LN formalism.

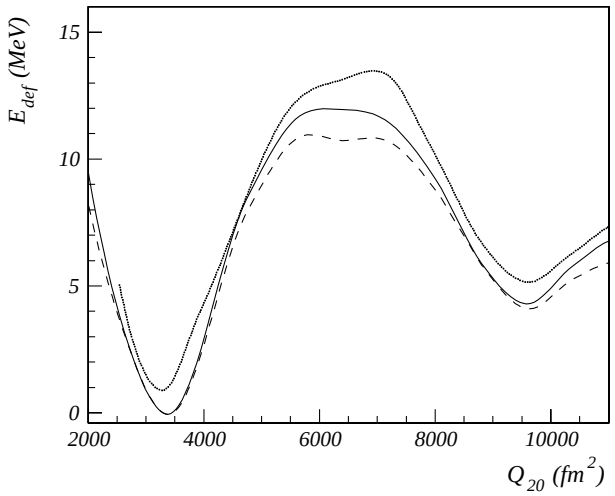

Fig. 4. Deformation energy curves are plotted as functions of the quadrupole moment Q_{20}. From bottom to top, dashed line corresponds to HFB calculation at zero spin, while full line (dotted, respectively) corresponds to HFB + LN calculations at zero spin (12 $\hbar$, respectively). The energy reference is taken as the unconstrained zero-spin energy value in both formalisms.

and $N = 152$ (see fig. 5 in [19]), we get only a comparable $N = 152$ gap plus a $N = 170$ gap at low spins which is not present in the paper of Duguet *et al.*.

In fig. 4 we display the fission barriers obtained at zero total angular momentum within the HFB and HFB + LN approaches allowing triaxial deformation. The former yields a first fission barrier which is slightly lower than what is obtained for the latter. Comparing HFB + LN results now for two different total angular momenta $I = 0\ \hbar$ and $I = 12\ \hbar$, we find that the first fission barrier height is slightly increased by 500 keV where one would expect it to be decreased. This phenomenon is due to a higher single-particle level density at the top of the first barrier for $I = 12\ \hbar$ as compared to what is obtained at zero spin. At such low spins, shell structure effects are thus able to mask the anti-binding effect of the rotation leading to an extra fission instability. With the basis size in use in our calculations we are not *a priori* able to provide reliable relative energies in the second fission barrier region, as noted years ago [28].

To conclude, it appears that the SkM* parameterization of the Skyrme interaction (complemented by a seniority force in the p-p h-h channel) is able to provide a good reproduction of the spectroscopic data in the ground-state rotational band of the ^{254}No nucleus within the HFB plus Lipkin-Nogami approach. This result is all the more remarkable that similar calculations [19] using a different effective force and yielding a rather different shell structure in the relevant deformation range, lead to a similarly (may be slightly less) good reproduction of the experimental data. Even though it is true that reproducing such collective rotation data provides a much wanted test of effective forces to be used when predicting the stability properties of neighbouring superheavy nuclei, such a convergence of results from seemingly rather different effective forces should mitigate the hope to get so far here a completely stringent benchmark.

The calculations of ref. [23] have studied in detail the fission properties of this nucleus, namely they underline its remarkable, and somewhat unexpected, fission stability which could partly be explained by a change of saturation properties of nuclear matter in presence of a centrifugal field as advocated in ref. [5]. Our results, limited in both spins and deformations as compared to those of ref. [23] yield similar conclusions on this stability. A pending point common to all these calculations (those of refs. [19,23] as well as ours) is the pairing correlation treatment in weak pairing regions as encountered upon increasing the angular velocity. Surely, treatment of such correlations within an approach that explicitly conserves the particle number, as the one proposed in refs. [26,27], would greatly improve the validity of the results.

However, whatever their mid stream character, the rather satisfactory reproduction of the difficult, and for that reason somewhat scarce, experimental results so far obtained by self-consistent calculations as those of refs. [19,23] and the one presented here, should constitute an incentive to experimentalists to provide more data so as to improve our knowledge of the effective interaction to be used. This certainly constitutes a very timely endeavour.

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