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Equilibrium deformations of rotating nuclei in a selfconsistent semiclassical approach

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Abstract: We study here equilibrium deformations of rotating nuclei within a selfconsistent semiclassical cranking approach using the SkM* Skyrme effective interaction. The different axial rotational configurations, i.e. where the rotation axis is parallel or perpendicular to the symmetry axis, are studied as well as the Jacobi bifurcation into triaxial rotational equilibrium shapes. Finally the validity of the concept of a rotating liquid drop which has been widely used for the determination of average shapes of rotating nuclei is assessed by comparison with our microscopic results.

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Abstract: We study here equilibrium deformations of rotating nuclei within a selfconsistent semiclassical cranking approach using the SkM* Skyrme effective interaction. The different axial rotational configurations, i.e. where the rotation axis is parallel or perpendicular to the symmetry axis, are studied as well as the Jacobi bifurcation into triaxial rotational equilibrium shapes. Finally the validity of the concept of a rotating liquid drop which has been widely used for the determination of average shapes of rotating nuclei is assessed by comparison with our microscopic results.

It has been known for a very long time that composite rotating objects at equilibrium experience various shape transitions upon increasing their angular velocities [1]. This is also the case for finite quantal objects like atomic nuclei, as studied extensively in Ref. [2] within the Liquid Drop Model (LDM). Further refinements of the standard LDM approach have dealt with situations where the nuclear shape is creviced or with the cases of quasi-molecular configurations [3,4]. On the other hand, semi-quantal calculations using the cranking or routhian approximation have been tackling the same problem either in a microscopic-macroscopic type of approach [5] or in a Hartree-Fock-Bogolyubov framework using rather realistic parametrizations of the effective

nucleon-nucleon force [6].

In the present work we will use a purely microscopic approach to study the bulk shape properties of rotating nuclei. Beyond the display of rotational properties associated with a given effective force, we aim at assessing the validity of more phenomenological approaches. To be specific, we want to test LDM-like calculations as well as macroscopic-microscopic calculations using the latter as a baseline for their energy evaluations within a Strutinsky framework. Two questions should indeed be raised about the use of the LDM in such a context: i) are there selfconsistent effects affecting in a significant fashion the density profiles as functions of the angular velocity, ii) more generally is the concept of a rotating liquid drop supported at all by microscopic calculations starting from a two-body effective force?

Our theoretical approach may be outlined as follows. We start from an effective interaction of the Skyrme type, whose capacity to describe static and low-energy dynamical properties is well established since many years [7]. More specifically, we will use here the SkM* parametrization [8]. Rotating nuclei will be described within the well-known semi-quantal cranking approximation which consists in minimizing the so-called routhian R :

$$\delta(R) = \delta < H - \boldsymbol{\omega} \cdot (\boldsymbol{\ell} + \boldsymbol{s}) > \tag{1}$$

where H is the effective nuclear Hamiltonian and ℓ (s resp.) the total orbital (spin resp.) angular momentum. Instead of determining the quantal variational solution of eq. (1), we rather consider its semiclassical approximation (where semiclassical is to be understood *à la Wigner*) within the so-called Extended Thomas-Fermi (ETF) approach [9], as described in a previous paper [10], hereafter referred to as I.

In I, explicit functional expressions for all the various densities entering the routhian density associated to a Skyrme force [11] have been derived in terms of the local (spin-scalar) density $\rho(r)$. To evaluate the latter at equilibrium, one should minimize the variational quantity of eq. (1) for a given value of ω within a restricted set of densities $\rho(r)$ which will be specified below. It is worth noting however, that we rather require here that the total angular momentum has a given value $I\hbar$

$$I\hbar = \frac{1}{\|\omega\|} < \boldsymbol{\omega} \cdot (\boldsymbol{\ell} + \boldsymbol{s}) > \tag{2}$$

This leads to performing many variational calculations corresponding to an adequate scanning of ω values in order to get the desired value of I. In what follows we have satisfied the eq. (2) with an accuracy better than $5 \cdot 10^{-3}$.

For the densities $\rho(r)$ we have chosen the family of modified Fermi functions given by (q standing for each one of the two charge states) :

$$\rho_q(r) = \rho_{0q} \left[1 + e^{\ell_q(r)/\alpha_q}\right]^{-\gamma_q} \tag{3}$$

where the function $\ell_q(r)$ is the distance from a generating surface as discussed in ref. [12].

As for the deformation space we will only consider in the present work, axial and triaxial ellipsoidal shapes, precluding thus a priori a realistic description of large deformations. For each charge state, we have thus considered four monopole parameters (ρ_{0q}, α_q, γ_q and a radius parameter) plus two deformation parameters. To keep contact, at least for moderate deformations, with usual shape parametrizations, we have labelled somewhat arbitrarily, our ellipsoidal shapes by the standard quadrupole parameters β and γ equating the semi-axis lengthes of the ellipsoids with the comparable lengthes of a standard quadrupole drop. Taking into account the conservation of the neutron and proton numbers and varying separately the monopole parameters of both charge states while imposing the same deformation to the two charge distributions, we are left with eight independent variational parameters.

According to I, the total Skyrme Hamiltonian expectation value associated with a solution which is not even with respect to time-reversal, can be written as

$$E = \int H_{sc}^{te}(\rho)\, d^3r + \frac{1}{2}\mathcal{I}(\rho)\,\omega^2 \tag{4}$$

where H_{sc}^{te} is the semiclassical Skyrme hamiltonian density associated with a time-even solution (see I) and $\mathcal{I}(\rho)$ is given as an integral of a quantity involving only ρ [13]. Whereas $\mathcal{I}(\rho)$ as seen in eq. (4) is clearly identified as the dynamical moment of inertia $\mathcal{I}^{(2)}$, it has been shown [13] that in our approach, this moment is identical to the kinematic moment defined as :

$$\mathcal{I}^{(1)} = \frac{\| < \boldsymbol{\ell} + \boldsymbol{s} > \|}{\|\boldsymbol{\omega}\|} \tag{5}$$

This result is not trivial since in eqs. (4,5) one has to take into account the ω-dependence of the many-body wawefunctions which are solutions of the variational problem and hence such a ω-dependence for ρ. One therefore gets the equilibrium solutions at a given value of the angular momentum $I\hbar$ by minimizing the laboratory energy E given in eq. (4). The numerical evaluation of this energy has been made upon using, after minor modifications, an ETF

triaxial code written by J. Libert [14]. As a matter of fact, the first (and numerically most important) term in eq. (4), has been evaluated to order four in $\hbar$ whereas the rotational energy term involving the moment of inertia $\mathcal{I}(\rho)$ has been evaluated as in paper I to second order only.

We will first discuss our results in the small ω-regime which could be named the Newton's regime in reference to the well-known axial oblate terrestrial-like solutions which are classically expected there. On Figure 1, the laboratory energy E is plotted for ^{56}Ni (at $I = 40$), ^{90}Zr (at $I = 40$ and 50) and ^{208}Pb (at $I = 60$), as a function of the axial deformation parameter β defining the ellipsoidal shape (as usual, β takes here a negative value for oblate shapes). One finds that indeed the lowest equilibrium solutions are oblate and have coinciding symmetry and rotation axis. However other local equilibrium solutions (higher in energy) are found on the prolate side ($\beta > 0$) in which case the symmetry and rotation axis are perpendicular. It is important to realize that, the angular momentum being fixed in such curves, the ω-values are changing with β, since

$$I\hbar = \mathcal{I}(\beta)\,\omega(\beta) \tag{6}$$

One finds in fact that $\omega(\beta)$ varies almost linearly near the spherical point as a function of β. Indeed as we will see below, a reasonably good representation at small deformations of $\mathcal{I}$ considered as a function of β, is provided by the rigid body formula which indeed exhibits there a linear dependence in β (see e.g. ref. [15].

For a nucleus whose charge and mass numbers are below some critical values, one reaches upon increasing ω, a point where triaxial ellipsoidal shapes correspond to the lowest solutions in energy. The advent of such a transition, dubbed as the Jacobi bifurcation point is displayed for ^{90}Zr in Figure 2 where the (β, γ) parameters of its most stable equilibrium solutions are reported as functions of I. With the convention for the γ-angle given in ref. [16], a solution with $\gamma = 60^o$ corresponds to axial oblate parallel rotations whereas $\gamma = 0^o$ refers to axial prolate perpendicular rotations. In between, we are considering rotations whose axis is the principal axis of the ellipsoid with the shortest semi-axis length. It is seen on Figure 2 that the Jacobi bifurcation occurs in ^{90}Zr between $I = 50$ and $I = 55$. Then up to $I = 60$, the equilibrium solution remains close to $\gamma \simeq 60^0$, while the laboratory energy surface is rather flat in the vicinity of the axial oblate edge. Suddenly for $I \geq 63$, the equilibrium solution moves away very rapidly with I, towards a perpendicular prolate type of rotation (see Figure 2). Ultimately for even higher values of I, one would reach a point of fission instability which we are unable to describe presently within our very limited shape parametrization space as above discussed.

A striking way of presenting this rather sudden transition from oblate parallel rotations with $\beta \simeq 0.3$ to prolate perpendicular rotations with $\beta \simeq 0.6$ (or higher), is to use a standard $\mathcal{I}/\hbar^2$ over $\hbar\omega$ plot where as usual

$$\hbar\omega = \frac{dE}{dI} \tag{7}$$

One gets indeed on Figure 3 a very nice backbending pattern, with the somewhat peculiar character though, of being purely semiclassical in nature (very much similar to what was found earlier, see Figure 4 of ref. [16]). It corresponds roughly to a band transition from a low deformation (low $\mathcal{I}$) to a large deformation (large $\mathcal{I}$) which is in fact in our case not at all stabilized, due to the fission instability. Indeed, around $I = 60$, the equilibrium solution increases its angular momentum by an increase of its moment of inertia (through its deformation) while keeping its angular velocity roughly constant.

It may appear that the above discussed results are rather similar, at least qualitatively, with those obtained in the rotating LDM [2,16]. It remains however to check the validity of the latter model: i) are LDM energies good representations of semiclassical ones ? ii) if so, are the LDM parameters ω-dependent ? We will devote the last part of this paper to provide answers to these questions. To do so, we have performed self-consistent semiclassical calculations for 33 different nuclei within and far out the β-stability valley, sampling roughly the whole chart of nuclides between the neutron and proton drip lines, excepting only very light nuclei where the LDM validity is dubious. The nuclei which have been considered are :

^{36,40,44,48,50}Ca, ^{56}Ni, ^{90}Zr, ^{100,104,108,110,114,118,122,126,130,132}Sn, ^{140}Ce, ^{168}Yb, ^{186}Os, ^{186,190,192,196,200,204,206,208,212,216}Pb, ^{230}Th, ^{240}Pu and ^{252}Cf.

We will merely discuss here the strong interaction part of the LDM energies written with usual notation (with $I = (N - Z)/A$) as

$$E = a_V(1 - k_V I^2)A + a_S(1 - k_S I^2)A^{2/3} \tag{8}$$

For that, on has to remove from the first term in the r.h.s. of eq. (4), the Coulomb (direct and exchange) energies even though they are of course included in our variational calculations and play indeed a crucial role for the symmetry energy properties discussed below through Hartree-Fock-like neutron-proton self-consistent effects.

To disentangle genuine variations of the LDM parameters with ω from purely geometrical deformation effects, we have first constrained all the nuclei to be spherical. Self-consistent semiclassical calculations have been performed

at seven $\hbar\omega$-values ranging from 0 to 1.2 MeV by steps of 0.2 MeV. First, one notices (see Table 1 for some selected nuclei) a significant variation of the bulk part of the nuclear energy with ω at least for large enough values of ω. This fact leads immediately to the conclusion that if the LDM is of any relevance in the rotating case, its parameters should vary to some extent with the angular velocity. There exists a large difference in the variations of the ETF energies from light nuclei (e.g. ^{40}Ca) to heavy nuclei (e.g. ^{208}Pb). However these variations are found to be of the same order of magnitude when multiplying them by $A^{5/3}$, i.e. considering these variations as functions of the angular momenta rather than of the angular velocities.

We have performed for all ω-values, a least-square fit of our calculated energies by the LDM formula given in eq. (8). The results are displayed in Table 2. It is first to be noted that the overall quality of the fit is nearly constant for the whole range of ω values, with a mean quadratic deviation of about 500 keV. Therefore within this error bar the validity of the LDM seems assessed, at least for spherical shapes. Upon increasing ω now, both the volume and volume symmetry energies change in the direction of a supplementary binding. The surface and surface symmetry energy terms, on the contrary, vary in the opposite direction. It is probable that the size of the sample used here does not permit to pin down with a large accuracy the relative variations of all four LDM parameters. Their consistent variations with ω however, seems to indicate that their binding or anti-binding characters and probably their absolute magnitudes up to $\simeq 0.1\,\%$ should be correct.

To give an idea of the error made when considering the LDM parameters as constant with respect to ω, it may be sufficient to stress that to change the ^{208}Pb binding energy by 1 MeV, one has to vary a_V by $-0.03\,\%$, $a_V k_V$ by $0.38\,\%$, a_S by $0.17\,\%$ and $a_S k_S$ by $-1.59\,\%$. This, of course, puts in proper perspective the rather high percentages obtained for the ω-variations of the symmetry LDM terms.

It remains now to check if what is fitted in the above as a surface term, varies indeed with the deformation as the surface of an ellipsoid. To achieve that, one has to substract from the nuclear energy the total volume contribution (i.e. with the symmetry term included) deduced from the previous fit. Similar checks could also be performed for the total Coulomb energy (disregarding a possible difference in the deformation dependence of the direct and exchange terms) and for the moment of inertia (or equivalently for the rotational kinetic energy). Due to the above discussed ω-variation of the LDM parameters, this is not a completely unambiguous task to accomplish. Indeed keeping contact with the approach of ref. [2] (dictated by the fact that the total angular momentum is a good quantum number), we have performed the above checks for given values of $I\hbar$. This implies thus to consider for different β-values different ω-values, and thence somewhat different LDM parameters. We will only

discuss here a typical example, namely the lowest axial deformation curves of ^{90}Zr for both oblate and prolate shapes at $I = 50$. On the oblate side for $\beta = 0.3$ for instance, the surface shape factor B_S of ref. [2] is underestimated by $\simeq 0.3\,\%$ in the LDM approach, whereas the Coulomb shape factor B_C is overestimated by $\simeq 0.2\,\%$ and the rotational shape factor B_R is underestimated by a larger amount, namely by $\simeq 2.5\,\%$. On the prolate side now and for the same value of β, the sign of the discrepancies are identical to what was obtained on the oblate side with slightly lower absolute values, namely 0.2 %, 0.2 % and 1.7 %. All these discrepancies are steadily increasing (in absolute value) upon increasing the deformation.

To conclude, we will simply state first that our microscopic results are qualitatively consistent with the LDM results of Cohen, Plasil and Swiatecki [2]. In that respect, we had already estimated in I the level of accuracy of the Rigid Body ansatz for the moments of inertia. In the present work we have demonstrated that for small angular velocities and small deformations the LDM ansatz is roughly accurate as compared to our results. The latter stemming from an effective force which has proven its realistic character, constitute indeed a satisfactory microscopic reference. Whenever a high degree of accuracy is needed or at large β and/or ω values, one should not escape to perform a more refined description than the liquid drop model one. The present approach is certainly a candidate for such a description being both microscopically founded and reasonably tractable. However in its present form, it is very limited for large deformations. We are presently improving the shape variational space of our densities so as to allow an adequate description of the fission instability region.

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Table 1
Nuclear energies (in MeV) calculated in our selfconsistent approach to be compared with Liquid Drop Model energies for various nuclei as functions of the angular velocity given by the energy $\hbar\omega$ (in MeV).

$\hbar\omega$	0.0	0.4	0.8	1.2
^{40}Ca	−419.93	−419.94	−419.99	−420.04
^{90}Zr	−1029.11	−1029.40	−1029.42	−1029.80
^{140}Ce	−1623.39	−1623.60	−1624.09	−1624.84
^{208}Pb	−2421.71	−2422.13	−2423.36	−2425.15

Table 2
Variation of various Liquid Drop Model parameters (in MeV) defined in the text, as functions of the angular velocity given by the energy $\hbar\omega$ (in MeV). The mean quadratic deviation of the fitted energies (in MeV) are also displayed.

$\hbar\omega$	0.0	0.2	0.4	0.6	0.8	1.0	1.2
a_V	−15.477	−15.477	−15.486	−15.489	−15.496	−15.502	−15.520
		−0.06	−0.12	−0.14	−0.19	−0.22	−0.34
$-a_V\kappa_V$	28.129	28.112	28.072	28.038	27.860	27.694	27.675
		−0.06	−0.20	−0.32	−0.96	−1.55	−1.61
a_S	17.056	17.057	17.087	17.100	17.124	17.138	17.208
		0.00	0.18	0.25	0.40	0.48	0.89
$-a_S\kappa_S$	−39.962	−39.837	−39.463	−39.293	−38.520	−37.538	−37.250
		0.31	1.25	1.67	3.61	6.07	6.79
$\sqrt{<\Delta E^2>}$	0.55	0.54	0.57	0.51	0.51	0.55	0.47

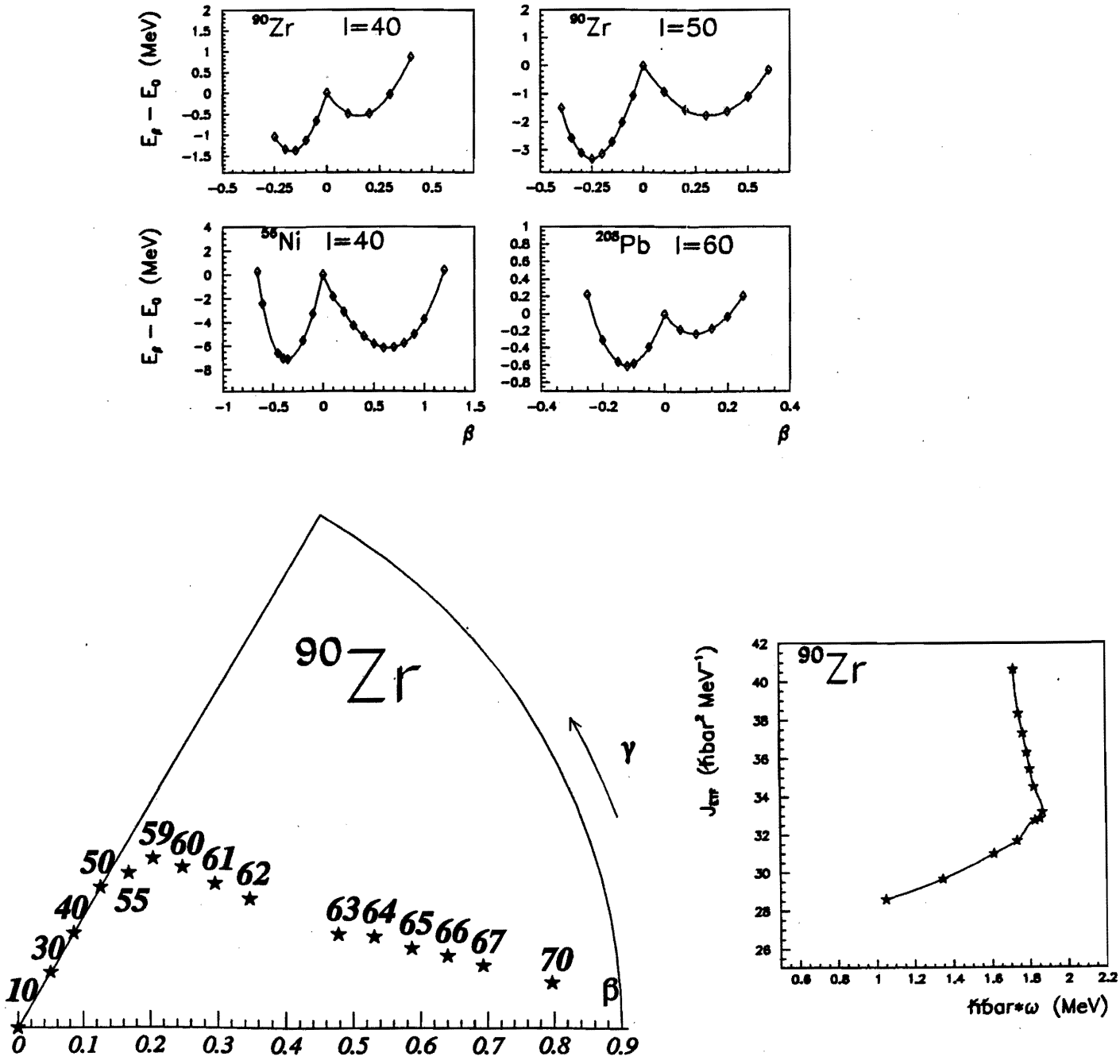
Figure captions

FIGURE 1

Deformation energies (in MeV) relative to the energies at sphericity for various nuclei and various values $I\hbar$ of the angular momentum.

FIGURE 2

Evolution in the (β, γ) plane of equilibrium solutions of ^{90}Zr as functions of the angular momentum parameter I.

FIGURE 3

Calculated ETF moment of inertia J_{ETF} (in $\hbar^2\, MeV^{-1}$) of ^{90}Zr as a function of the rotational energy $\hbar\omega$ (in MeV).