## **Rotational states and masses of heavy and superheavy nuclei**

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The macroscopic-microscopic model with the Lublin-Strasbourg drop, the Strutinsky shell-correction method, and the BCS approach for pairing correlations is used with the cranking model to describe nuclear masses and rotational bands in even-even Ra to Cn isotopes of actinide and transactinide nuclei. The single-particle levels and potential-energy surfaces are calculated with the Yukawa-folded single-particle potential using the "modified funny hills" (*c*, *h*) shape parametrization. A monopole pairing force is used in our calculations. At equilibrium deformation the pairing strength is adjusted for every nucleus so as to reproduce the experimentally known rotational  $E_{2+}$  state within the cranking model. The pairing strength obtained in this way is used to predict the masses and rotational states in superheavy No to Cn nuclei. It is also shown that the rotational states with  $L\lesssim 10$ in Ra to No nuclei evaluated using a simple rotational formula agree quite well with the data. We propose a simple mechanism which takes into account a dynamical coupling of rotation with the pairing field that then allows one to obtain an excellent agreement with the data up to the states with the largest angular momenta ( $L \leqslant 30$ ) measured in this mass region.

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# **I. INTRODUCTION**

Experimentally known rotational  $E_{L^+}$  states (up to  $L = 30$ ) of even-even Ra to No isotopes [\[1,2\]](#page-6-0) are investigated within the rotational model using the cranking moment of inertia [\[3\]](#page-6-0). The potential-energy surfaces of these nuclei are obtained using the macroscopic-microscopic method with the Lublin-Strasbourg drop (LSD) [\[4\]](#page-6-0) and the Strutinsky shell-correction method [\[5\]](#page-6-0), evaluated on the basis of a Yukawa-folded (YF) meanfield potential [\[6\]](#page-6-0). Pairing corrections are calculated within the BCS approach [\[7\]](#page-6-0) with the pairing strengths adjusted for every nucleus so as to reproduce the quadrupole  $E_{2+}$  rotational states found in the experiment. The pairing strength obtained for a given nucleus in this way is then used to write down a *Z*- and *N*-dependent expression for it. The equilibrium deformations are determined by minimizing the total energies on the twodimensional  $(c, h)$  grid of the "modified funny hills" (MFH) shape parametrization [\[8\]](#page-6-0), where *c* represents an elongation parameter and *h* measures the neck degree of freedom. The moment of inertia is shown to strongly depend on the pairing gap which leads to a contraction of the theoretical rotational spectra when one includes the coupling of the rotational and pairing degrees of freedom (see also Ref. [\[9\]](#page-6-0)). Our results turn out to be close to those of Ref. [\[10\]](#page-6-0). We have finally used our approach to predict the masses and  $E_{2+}$  energies of some superheavy nuclei.

## **II. THEORETICAL MODEL**

Nuclear energy is calculated within the macroscopicmicroscopic model [\[11\]](#page-6-0) with the LSD expression [\[4\]](#page-6-0) for macroscopic energy and the Strutinsky shell correction [\[5\]](#page-6-0) plus the BCS pairing-correlation energy for the microscopic part:

$$
E = E_{\text{LSD}} + E_{\text{corr}}.\tag{1}
$$

The microscopic correction needs to be determined separately for protons and neutrons,

$$
E_{\text{corr}} = E_{\text{shell}} + E_{\text{pair}} = E_{\text{shell}}^p + E_{\text{shell}}^n + E_{\text{pair}}^p + E_{\text{pair}}^n. \quad (2)
$$

The Lublin-Strasbourg drop energy is given as

$$
E_{\text{LSD}} = -b_{\text{vol}}(1 - \kappa_{\text{vol}}I^2)A + b_{\text{surf}}(1 - \kappa_{\text{surf}}I^2)A^{2/3} + b_{\text{cur}}(1 - \kappa_{\text{cur}}I^2)A^{1/3} + \frac{3}{5}e^2 \frac{Z^2}{r_0^{\text{ch}}A^{1/3}} - C_4 \frac{Z^2}{A} - C_0 \exp(-W|I|/C_0),
$$
 (3)

with the relative isospin  $I = (N - Z)/A$  and where the parameters have been obtained in Ref. [\[4\]](#page-6-0) by a fit to the known masses of 2766 isotopes:

$$
b_{\text{vol}} = 15.4920 \text{ MeV}, \quad \kappa_{\text{vol}} = 1.8601,
$$
  
\n
$$
b_{\text{surf}} = 16.9707 \text{ MeV}, \quad \kappa_{\text{surf}} = 2.2938,
$$
  
\n
$$
b_{\text{cur}} = 3.8602 \text{ MeV}, \quad \kappa_{\text{cur}} = -2.3764,
$$
  
\n
$$
r_0^{\text{ch}} = 1.21725 \text{ fm}, \quad C_4 = 0.91810 \text{ MeV},
$$
  
\n
$$
C_0 = 10 \text{ MeV}, \quad W = 42 \text{ MeV}.
$$

The deformation LSD energy is

$$
E_{\text{def}}^{\text{LSD}} = E_{\text{LSD}}(c, h) - E_{\text{LSD}}(1, 0). \tag{4}
$$

Note that  $(c=1, h=0)$  corresponds to the spherical shape. The total deformation energy is similarly

$$
E_{\text{def}}^{\text{tot}} = E(c, h) - E(1, 0). \tag{5}
$$

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<span id="page-1-0"></span>The shell-correction energy in Eq. [\(2\)](#page-0-0) is defined as the difference between the sum of single-particle (s.p.) energies *eν* and its average value

$$
E_{\text{shell}} = \sum_{\nu} e_{\nu} - \tilde{E}, \qquad (6)
$$

which is obtained from the sum of single-particle energies by a Strutinsky-averaging procedure [\[5\]](#page-6-0)

$$
\tilde{E} = 2 \int_{-\infty}^{\lambda} e\bar{\rho}(e) \, de,\tag{7}
$$

where the smoothed level density distribution is

$$
\tilde{\rho}(e) = \frac{1}{\gamma} \sum_{v} f\left(\frac{e - e_v}{\gamma}\right),\tag{8}
$$

with a smoothing function  $f(u)$  given by a Gaussian multiplied by a sixth-order correctional polynomial

$$
f(u) = \frac{1}{\sqrt{\pi}} e^{-u^2} \left( \frac{35}{16} - \frac{35}{8} u^2 + \frac{7}{4} u^4 - \frac{1}{6} u^6 \right). \tag{9}
$$

The smoothing width  $\gamma$  has to be chosen in such a way as to make the energy  $\tilde{E}$  of Eq. (7) stationary (fulfilling the so-called plateau condition) which is generally the case when choosing the smearing width slightly larger than the average major shell spacing  $\gamma = 1.2 \hbar \ \omega_0$ , with  $\hbar \ \omega_0 = 41/A^{1/3}$  MeV.

The Fermi level  $\lambda$  in Eq. (7) is determined by the particlenumber equation

$$
\mathcal{N} = 2 \int_{-\infty}^{\lambda} \tilde{\rho}(e) de, \qquad \mathcal{N} = \{N, Z\}.
$$
 (10)

The pairing correction energy is defined as the difference between the BCS energy evaluated at the minimum with respect to the variational parameters  $u<sub>v</sub>$  and  $v<sub>v</sub>$  and the sum of s.p. energies  $e<sub>v</sub>$  minus the average pairing energy [\[12\]](#page-6-0)

$$
E_{\text{pair}} = E_{\text{BCS}}^{\text{min}} - \sum_{\nu} e_{\nu} - \langle E_{\text{pair}} \rangle.
$$
 (11)

The BCS energy of a system with even number of particles and a seniority pairing force is given by [\[3\]](#page-6-0)

$$
E_{\rm BCS} = \sum_{\nu>0} 2e_{\nu}v_{\nu}^2 - G\left(\sum_{\nu>0} u_{\nu}v_{\nu}\right)^2 - G\sum_{\nu>0} v_{\nu}^4 ,\qquad(12)
$$

where  $v_y = \sqrt{(e_y - \lambda)^2 + \Delta^2}$  is the occupation probability amplitude of the pair  $\{|v\rangle, |-\nu\rangle\}$  with  $|-\nu\rangle$  being the timereversed of state  $|v\rangle$  and  $u_v = \sqrt{1 - v_v^2}$ . The parameters  $\Delta$  and *λ* are the pairing gap and Fermi energy, respectively. The minimum of the BCS energy  $E_{\text{BCS}}^{\text{min}}$  corresponds to  $\Delta_0$ , which one can evaluate from the coupled system of the gap and the particle number BCS equations [\[3\]](#page-6-0). The pairing strength *G* is the input parameter of the BCS theory and influences not only the energies but also the cranking moments of inertia.

The nuclear ground-state mass is obtained as

$$
M_{\rm th} = ZM_{\rm H} + NM_n - 0.00001433Z^{2.39} + E, \quad (13)
$$

where  $M_H$  is the mass of the hydrogen atom and  $M_n$  the neutron mass. The third term takes into account the effect of the electronic orbits, and *E* is the binding energy of Eq.  $(1)$ .

The cranking moment of inertia  $\lceil 3 \rceil$  is given by

$$
\mathcal{J} = 2\hbar^2 \sum_{\mu>0} \sum_{\nu>0} \frac{|\langle v|\hat{J}_x|\mu\rangle|^2}{E_\mu + E_\nu} (u_\mu v_\nu - u_\nu v_\mu)^2, \qquad (14)
$$

where  $\mu$  and  $\nu$  are labels of the s.p. states with quasiparticle energies  $E_{\mu}$  and  $E_{\nu}$ . The operator  $\hat{j}_x$  is the projection of the total s.p. angular momentum on the axis around which the rotation is performed in the intrinsic frame (*x* axis). The ground-state rotational band for the lowest angular momenta *L* can then be described by a simple rotational model:

$$
E_{L^{+}} = \frac{L(L+1)\hbar^2}{2\mathcal{J}}.
$$
 (15)

### **III. CALCULATION**

We have performed calculations as described above for 88 even-even nuclei from  $^{226}$ Ra up to  $^{278}$ Cn which are sketched in Fig. 1 in the  $(N, Z)$  plane. Isotopes with measured  $E_{2^+}$  states (between 226Ra and 254No) are denoted by crosses. Superheavy elements, where the rotational states  $E_{2+}$  are not yet known, are marked by circles. For these nuclei, a prediction of the masses and  $E_{2+}$  energies is given. The choice of this region is the same as the one of Ref. [\[10\]](#page-6-0). It contains deformed even-even nuclei which can exist due to shell corrections. Neutron separation energies for these nuclei are positive indicating that they are bound, and their rotational states should exist and be measured in the future.

Our calculations were performed with the MFH shape parametrization [\[8\]](#page-6-0) on a two-dimensional deformation mesh with elongation parameter *c* and neck parameter  $h: 0.8 \leq c \leq$ 1.6 and  $-0.4 \le h \le 0.4$ . The calculations are performed in the following steps:



FIG. 1. Nuclei investigated in the present paper: crosses indicate nuclei for which rotational states are measured, open circles superheavy nuclei for which masses and  $E_{2+}$  energies are predicted. The solid line corresponds to Green's *β* stability line.

<span id="page-2-0"></span>

FIG. 2. (Color online) Values of the pairing strength parameter  $g_0$  needed to reproduce  $E_{2^+}$  energies of even-even Ra to No isotopes.

(i) First the YF s.p. potential is diagonalized for each nucleus and the s.p. levels are obtained in every grid point of the deformation landscape.

(ii) The microscopic corrections are then determined making sure that the plateau condition of the Strutinsky method is well satisfied.

(iii) Following Refs.  $[13,14]$ , where the pairing strength for protons and neutrons were approximated by a formula  $G_p Z^{2/3} = G_n N^{2/3} \approx 0.3\hbar \omega_0$  with one constant only, we have chosen the following expression for the pairing strength in our model:

with the constant  $g_0$  in MeV (instead of  $\hbar \omega_0$  units) and with the constant  $g_0$  in MeV (instead of  $h \omega_0$  units) and assuming that the pairing window contains  $\sqrt{15N}$  s.p. levels closest to the Fermi surface.

In nuclei with experimentally known  $E_{2^+}$  energy, the theoretically determined *E*2<sup>+</sup> will, generally, not quite coincide with its experimental value. We therefore take the freedom to adjust, for each nucleus, the value of the pairing-strength parameter  $g_0$  in such a way that theoretical and experimental  $E_{2^+}$  agree perfectly. The resulting values of such pairing strengths are presented in Fig. 2. To these results one average *g*<sup>0</sup> was fitted.

(iv) Using this optimal pairing strength  $g_0 = 12.29$  MeV, the potential-energy surface of the nucleus is recalculated and the equilibrium deformation  $(c_{eq}, h_{eq})$  is determined. At the equilibrium point, the cranking moment of inertia is used to evaluate the rotational levels for different *L* values with the rotational formula  $(15)$ . No stretching effect is taken into account, since we have found that in this region of nuclei the equilibrium deformation stays almost the same with growing angular momentum. The rms deviation of the theoretical  $E_{2+}$ energies for all 39 investigated nuclei, where experimental data exist, is 1.8 keV only, as compared to a rms deviation of 4.1 keV for the 27 isotopes discussed in Ref. [\[10\]](#page-6-0).

In the following section we present a comparison of the obtained rotational energies with the experimental data and predict the positions of the  $E_{2+}$  states and the masses of superheavy nuclei.

## **IV. RESULTS**



Figure 3 shows for the nucleus  $^{238}$ Cm the different ingredients of the total deformation energy  $E_{\text{def}}^{\text{tot}}$ , namely, the



FIG. 3. (Color online) Energies and moments of inertia of <sup>238</sup>Cm on the *c*, *h* plane.

<span id="page-3-0"></span>

FIG. 4. Cross section of the potential energies *E* for 236U (top) and 238Cm (bottom) nuclei as function of the mass-asymmetry deformation parameter  $\alpha$  at the first and second minima.

Strutinsky shell-correction energy  $E_{shell}$ , the pairing energy  $E_{\text{pair}}$ , the sum of both microscopic corrections  $E_{\text{corr}}$  and the macroscopic deformation energy  $E_{\text{def}}^{\text{LSD}}$ , together with the cranking moment of inertia  $J$ . One notices that shell and pairing energies oscillate strongly with amplitudes of 10 and 5 MeV, respectively, but these corrections are almost in opposite phases, so the total correction energy fluctuates much less. The macroscopic LSD energy has a broad minimum around the spherical shape  $(c = 1, h = 0)$ , and the macroscopic saddle point is located 2.1 MeV above the ground state at deformation  $c = 1.4$  and  $h = 1$ , so the correction energy modifies this landscape dramatically. The total deformation energy of <sup>238</sup>Cm has two minima of comparable depth located, respectively, at  $(c = 1.175, h = -0.12)$  and  $(c = 1.427, h = 0)$ . The cranking moment of inertia grows rapidly with increasing elongation *c* and does not depend significantly on the neck parameter *h*. We have calculated the rotational energies and masses in the first minima for all nuclei.

All calculations presented here are made for shapes with reflection symmetry, since the majority of investigated nuclei have in the ground state a deformation  $\alpha = 0$  [\[15–17\]](#page-6-0). In Fig. 4 the cross section of the potential-energy surfaces in the *α* direction at the first and the second minimum are shown for  $236$ U and  $238$ Cm. In both cases the stiffness with the reflection asymmetry degree of freedom  $\alpha$  is smaller for the ground state than for the shape isomeric minimum.



FIG. 5. Rotational energies  $E_{L^+}$  of the <sup>248</sup>Cm nucleus. Experimental data  $(x)$  are taken from Ref. [\[2\]](#page-6-0). Estimates of a simple rotational model, Eq.  $(15)$ , are denoted by  $(○)$  and those of the dynamical model, Eq.  $(18)$ , by  $\bullet$ ). A standard average pairing energy  $E_0$  of 2.3 MeV is used.

For the above selected even-even Ra to No isotopes, the rotational energies are presented in Table [I](#page-4-0) for angular momenta up to  $L = 30$ . The  $E_{2^+}$  energies evaluated using the simple rotational  $L(L + 1)$  rule of Eq. [\(15\)](#page-1-0), denoted as "r" in the table, are compared with the experimental data "e" taken from Refs. [\[1,2\]](#page-6-0) and the energies "d" obtained taking into account the dynamical coupling of the rotation with the pairing mode as described by Eq. [\(18\)](#page-4-0) below. For a majority of investigated nuclei, a reasonably good agreement of the pure rotational estimates is obtained for angular momenta up to about  $L \lesssim 10$ . After that, at higher angular momenta and excitation energies, it appears that the simple rotational model does not work properly, as the experimental data no longer fulfill the  $L(L + 1)$  rule and the corresponding level scheme appears more stretched than the experimental one, as shown for the  $248$ Cm isotope in Fig. 5.

It is well known, however, that a rapid rotation influences the pairing correlation. We therefore propose here a simple model which allows us to explain this mechanism and obtain some more quantitative estimates. In a standard calculation, the ground-state pairing gaps for protons  $(\Delta_0^p)$  and neutrons  $(\Delta_0^n)$  are determined from the BCS equation, i.e., looking for the minimum with respect to  $\Delta^q$  ( $q = p$  or *n*) of the BCS energy of a nonrotating nucleus. From the cranking formula, one can show that in the absence of pairing correlations ( $\Delta^p$  =  $\Delta^n = 0$ ) the moment of inertia is approximately equal to the rigid-body moment of inertia  $\mathcal{J}_{\text{rig}}$  but decreases with growing  $\Delta$  [\[18,19\]](#page-6-0). Its  $\Delta$  dependence can be approximated by

$$
\mathcal{J}(\Delta) = \frac{\mathcal{J}_{\text{rig}}}{1 + a(\Delta/\Delta_0)^2}.
$$
 (17)

Here  $\Delta/\Delta_0$  corresponds to the line  $\Delta^p/\Delta_0^p = \Delta^n/\Delta_0^n$  on the  $(\Delta^p, \Delta^n)$  plane, where, as above,  $\Delta_0^p$  and  $\Delta_0^n$  are the groundstate pairing gaps, and  $a = \mathcal{J}_{\text{rig}}/\mathcal{J}_0 - 1$  with  $\mathcal{J}_0$  the groundstate cranking moment of inertia. Such a dependence of the moment of inertia reflects in the rotational energy [\(15\)](#page-1-0) which being inversely proportional to  $\mathcal{J}(\Delta)$  grows with  $\Delta$  and shifts the minimum of the BCS energy toward smaller  $\Delta$ . This effect

<span id="page-4-0"></span>



is illustrated in Fig. 6, where the sum of the BCS and rotational energy

$$
E_{\rm BCS}^{\rm R}(\Delta; L) = E_{\rm BCS}(\Delta) + \frac{\hbar^2 L(L+1)}{2\mathcal{J}(\Delta)}\tag{18}
$$

relative to the BCS ground-state energy  $E_{BCS}(\Delta_0)$  is plotted as a function of  $\Delta/\Delta_0$ . The dependence of the BCS energy on  $\Delta$  is approximated by a cubic form

$$
E_{\rm BCS}(\Delta) = E_0 \left[ -3 \left( \frac{\Delta}{\Delta_0} \right)^2 + 2 \left( \frac{\Delta}{\Delta_0} \right)^3 \right],\tag{19}
$$

where  $E_0 = -\langle E_{\text{pair}} \rangle \approx 2.3 \text{ MeV}$  is the absolute value of the average pairing correlation energy [\[20\]](#page-6-0).

It is seen in Fig. 6 that the energy minima (black points) corresponding to  $L = 20$  and  $L = 30$  are significantly shifted down in comparison with the pure rotational-model estimates (open circles). This dynamical coupling of rotation with the pairing field brings the theoretical estimates to the experimental data as illustrated for  $248$ Cm in Fig. [5.](#page-3-0) Such an effect of

a dynamical coupling of the rotation with the pairing mode is taken into account for the estimates denoted by "d" in Table I, where the longest  $(L_{\text{max}} > 10)$  rotational bands in



FIG. 6. Energy gap dependence of the pairing and rotational energy.

![](_page_5_Figure_1.jpeg)

FIG. 7. (Color online) Mass discrepancies for Fm to Hs isotopes as functions of neutron number *N*.

the region were shown. Let us insist here on the fact that not a single parameter is adjusted to the data. As can be seen in Fig. [5](#page-3-0) these dynamical estimates are, indeed, close to the experimental data, even for the levels with the largest measured angular momenta, which proves that the coupling of the rotation with the pairing mode is important and should be taken into account in future calculations. All data presented in Table [I](#page-4-0) are evaluated without taking into account the change of the equilibrium deformation with growing angular momenta, since in this region of nuclei this effect is smaller than the one described above.

Nuclear masses are a good test ground for the quality of the model used to determine them, in particular for such different ingredients as the nuclear deformation energies or the pairingenergy strength. The deviations of the nuclear masses from the experimental data are presented in Fig. 7 for the heaviest elements Fm to Hs, where experimental data exist. The rms deviation for the 17 isotopes presented here is 0.29 MeV as compared with the LSD [\[4\]](#page-6-0) rms deviation of 0.41 MeV for the same sample of nuclei. It is seen that the difference between experimental and theoretical masses (evaluated with the pairing strength adjusted to the  $E_{2+}$  energies rather than to the experimental mass differences) does not exceed 0.6 MeV.

![](_page_5_Figure_5.jpeg)

FIG. 8. (Color online) Theoretical and experimental masses for No to Cn isotopes as functions of neutron number *N*.

![](_page_5_Figure_8.jpeg)

FIG. 9. (Color online) Theoretical rotational energies  $E_2^+$  for No to Cn isotopes as functions of neutron number *N*.

Such a good result encourages us to predict the masses for other superheavy nuclei. The result is shown in Fig. 8. To compare with the results of our calculations, only a few experimental masses are known in this superheavy region. They are denoted by crosses or boxes and agree rather well with our predictions.

We have used also our model with the pairing constant  $g_0 =$ 12.29 MeV to predict  $E_{2^+}$  energies of a series of No up to Cn superheavy nuclei. The trend for different isotopic chains is shown in Fig. 9. We find  $E_{2+}$  energies in the range between 30 and 70 keV, as compared to a range between 40 and 60 keV given in Ref. [\[10\]](#page-6-0).

### **V. CONCLUSIONS**

The deformation energies obtained for 88 even-even actinide and transactinide nuclei between Ra and Cn generally show a deep, well-deformed first minimum and, in some isotopes, a second minimum is also found. The location of the potential-energy minimum turns out to be weakly dependent on higher angular-momentum values and not too large deviation of the pairing strengths.

Parallel to the standard way of fixing the pairing constant *g*<sup>0</sup> [Eq. [\(16\)](#page-2-0)] from the mass difference of neighboring isotopes  $(Z = \text{const})$  and isotones  $(N = \text{const})$  which gives in this region of nuclei [\[14\]](#page-6-0)  $g_0^p = 12.26$  MeV for protons and  $g_0^n =$ 11.77 MeV for neutrons, we have obtained the value of  $g_0 =$ 12.29 MeV by reproducing the  $E_{2+}$  rotational energies when assuming  $g_0^p = g_0^n = g_0$ . Such value of  $g_0$  was used to foresee the rotational and binding energies of superheavy nuclei, where such energies have not yet been measured.

This alternative method is especially suitable in the heaviest nuclei region, where the chains of known isotopes and isotones are rather short and one cannot effectively use the four-point mass difference formula. The estimates of the binding energies of the heaviest nuclei (see Fig. 7) evaluated with *g*<sup>0</sup> fixed to positions of the lowest  $E_{2+}$  states are close to the experimental values, which in our opinion validates the new method. Generally, one can say that the pairing strength adjusted to  $E_{2+}$  positions reproduces well the binding energies in all cases where one deals with good rotors, which is the case in very heavy nuclei.

<span id="page-6-0"></span>The pure rotational model used to evaluate the excitation energies of the rotational band gives a nice agreement with the experimental data for the lowest rotational states up to  $L = 10$ , wherever such data exist; but for the larger angular momenta, the agreement becomes worse. We have shown that to obtain a reasonable description for higher angular-momentum states requires taking into account the dynamical coupling of the rotation with the pairing field.

To obtain a still better description of the rotational states with  $L > 10$ , we are planning to perform a minimization

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procedure for every spin independently in a four-dimensional space composed of the MFH  $(c, h)$  deformation parameters and the pairing gaps  $\Delta^p$  and  $\Delta^n$ .

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