THEORETICAL SURVEY OF SUPERHEAVY ELEMENTS*

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(Received November 12, 2013)

Half lives of superheavy elements are discussed. Energies were obtained in the framework of Skyrme Hartree–Fock–Bogoliubov (HFB) theory and the mass parameters in adiabatic time dependent HFB (ATDHFB) cranking approximation. The SkM* energy density functional (EDF) was used in the particle–hole channel and density dependent delta interaction (DDDI) in a mixed form in the particle–particle channel. Ground state energies were estimated on the semi-classical WKB formula resembling the Bohr– Sommerfeld (BS) quantization rule. The results for spontaneous fission, alpha and beta decays are presented and discussed. The most stable superheavy nuclei are located in the vicinity of Z = 112, N = 182.

DOI:10.5506/APhysPolB.45.273 PACS numbers: 24.75.+i, 25.85.Ca, 21.60.Jz, 27.90.+b

1. Introduction

In our previous paper [1] on the stability of superheavies (SH), we discussed a model of spontaneous fission whose ground state energy was estimated on the basis of rather exact calculations [2]. The energy was assumed to be equal to $E_0 = 0.7 E_z$, where E_z is a zero point energy at the ground state. E_z was calculated according to generator coordinate method (GCM) [3] with the mass parameters replaced by the ATDHFB cranking masses. The obtained half lives (HL) deviated from the observed ones by few orders of magnitude in the so-called *critical region* of $Z \approx 172$ where some SH nuclei were found experimentally [4].

The goal of the present calculations is to improve the results of our early estimates taking into account two facts. First, as it was mentioned in many places (see *e.g.*, [5, 6] where the rotational moment of inertia — a part of

^{*} Presented at the XXXIII Mazurian Lakes Conference on Physics, Piaski, Poland, September 1–7, 2013.

inertia tensor is discussed) — the ATDHFB cranking mass is too small in comparison to the full ATDHFB one. The authors of the paper use rather the scaled inertia parameters and the scaling factor 1.3 is applied. We follow this principle in the presented paper. Second, the approximation we have used in calculations of E_0 was rather crude and in the following we use some other recipe consistent with WKB approximation which is usually used to calculate the spontaneous fission probability. We shall treat this issue in Section 2.

2. Theory

The calculation of main ingredients of the theory, namely the potential energy and the mass parameter were described elsewhere [3, 7]. Processes β^{\pm} and electron capture were treated according to Ref. [8].

Calculating the energies, we assumed one leading coordinate (constraint) which is the mass quadrupole moment of the system $q_2 = \langle \hat{Q}_{20} \rangle$ and two other constraints namely the nonaxiality and the mass asymmetry which were applied in the region of the first barrier and in the region behind the barrier respectively. The detailed discussion is given in our previously published papers [3, 7]. In the following, we only discuss some new assumptions concerning the spontaneous fission process.

The ground state energy measured relatively to the minimum of the potential energy is a crucial parameter in determining the HL of the nucleus with respect to fission. The approximate fission probability P stemmed from WKB theory consists of mass parameters \mathcal{M} , potential energy V and the energy of the ground state of the system E_0 . In the approximation, the wave function as usual is assumed to be continuous at classical turning points. It means the following condition should be fulfilled [9]

$$\int_{a}^{b} \sqrt{2\mathcal{M}(q)(E_0 - V(q))} \, dq = \pi (n + 1/2)\hbar, \qquad (1)$$

where q is leading collective coordinate towards fission, n = 0, 1, ..., and a and b are the classical turning points determined from the equation $V(q) = E_0$ solved in the vicinity of the ground state. Equation (1) is similar to the Bohr–Sommerfeld quantization rule (see e.g., [10]). It can be easily solved for each considered nucleus with respect to E_0 . While the fission probability P strongly depends on E_0 , the results of calculation will be different from those where one assumes $E_0 = 0.5$ MeV (see e.g. [5, 11]) — a constant for all of nuclei.

As it was pointed out in the introductory section, the ATDHFB cranking mass parameters are on the average smaller then full ATDHFB ones. Therefore, to do more realistic calculations of fission HL, we assumed according to other authors the scaled fission mass tensor component. The scaling factor 1.3 was applied. This leads, in general, to larger values of E_0 (see Eq. (1)) and because of larger mass parameters at the same time to longer fission HL.

Before we proceed, we demonstrate the validity of the applied procedure and check its agreement in the known case of fermium isotopes for which very exact data exist. The results are shown in Fig. 1. There are shown decimal logarithms of experimentally known HL (crosses), results of our previous calculations (open circles, s7) and the results of a new procedure just described (BS-1.3). The root mean square error (r.m.s.) for the new evaluation is r.m.s. = 0.81 and the maximal deviation $\delta = \max |T^{\text{th}} - T^{\exp}| = 0.68$. The very peculiar systematics of experimental data is well reproduced by the theoretical calculation. The bottom panel in Fig. 1 shows the ground state energies as calculated previously and using WKB quantization condition with n = 0 which corresponds to the ground state.



Fig. 1. (Color online) Decimal logarithms of fission HL (in seconds) of fermium isotopes. Crosses correspond to experimental data, open circles (blue) are the old results with scaled $E_0 = 0.7 E_z$ and filled circles (red) are the new results based on the ground state energy E_0 calculated from WKB quantization formula of Eq. (1). The bottom panel shows corresponding ground state energies [MeV]. The r.m.s. error and the maximal deviation $\delta = \max |T^{exp} - T^{th}|$ are shown for the case of BS-1.3 model.

3. Results

In Fig. 2 we show decimal logarithms of the spontaneous fission HLs (seconds). The longest calculated HL (model BS-13) characterize nuclei with $N \sim 182 \pm 2$ and $Z \sim 118 \pm 4$. The values of $T_{\rm sf}$ are $\sim 10^{12}$ seconds.



Fig. 2. (Color online) Decimal logarithms of spontaneous fission HL (Models BS-13 — present paper (left panel), and s7 — the past results of Ref. [3] (right panel).

The inclusion of the alpha decay into consideration changes the described stability picture. Figure 3 shows combination of spontaneous fission and α -decay HL of SH. One can observe the reduction of the longest fission HL in the region of $N \sim 182 \pm 2$ and $Z \sim 118 \pm 4$ by many orders of magnitude. The stability island is located at $N \sim 182 \pm 2$ and $Z \sim 110 \pm 2$. The longest HL is shorter then one year.

Figure 4 shows the total HL including all modes of decay: α , β and SF and the probabilities of these processes. The longest total HL correspond to nuclei in the vicinity of Z = 112 and N = 182-184. The values of HL are of the order of 10^4 seconds. The dominant processes in the considered region of nuclei are both the α decay and the spontaneous fission. The nuclei with $Z \leq 114$ and N = 182, 184 undergo the beta decay. The lighter nuclei (A < 280) undergo fission in a symmetric way, while the heavier one prefer an asymmetric mode — division into two asymmetric fragments. There are two regions of superheavies one at N = 164, Z = 112 and another one at N = 182, Z = 120 which decay by the alpha emission. On the borders of all of the regions all of the decay processes concur one with each other.



Fig. 3. (Color online) Decimal logarithms of both alpha decay and spontaneous fission half lives (Model BS-13, see the text).



Fig. 4. (Color online) Plot of HL (decimal logarithms are proportional to the circle radius) and the decay modes probabilities of SH nuclei: symmetric fission (light grey/orange), asymmetric fission (grey/green), alpha decay (dark grey/red) and total beta decay (black/navy). The corresponding probabilities are proportional to an angle of the circle sectors. The (squares/blue) squares depict the experimentally observed even–even SH elements.

4. Summary and outlook

In the paper, we have shown the HL of SH nuclei and discussed the elementary decay modes (spontaneous fission, alpha and beta processes). Superheavy nuclei undergo all types of elementary processes and all of them are important in different regions of nuclear chart of superheavies. There exist regions where one observes a symmetric fission (light nuclei) or asymmetric one (heavy elements), the alpha decay (both light and heavy SH elements) and also the beta decay (heavy, $Z \sim 112 \pm 2$, $N \sim 182$).

The WKB quantization rule which delivers the ground state energy E_0 for fission works well at least in the region of known elements as *e.g.*, in the case of fermium isotopes. Its extrapolation to SH elements seems to be better than an *ad hoc* procedure which was assumed previously, where the ground state energy E_0 was equal to $0.7 E_z$ or it was constant equal to 0.5 MeV.

According to our calculations, the longest total half lives correspond to nuclei in the vicinity of Z = 112 and N = 182, 184. The inclusion of all decay channels (β^{\pm} , electron capture, α and spontaneous fission) shifts the stability region predicted in other papers from Z = 124 and 126, N = 184to $Z \sim 112$, $N \sim 182$, 184. This is one of the main conclusion of the paper.

There are, of course, discrepancies between the theoretical and the experimental data, the largest ones in the region of the middle mass SH nuclei. Since those systems belong to the region of shape coexistence some further increase of SF HL is anticipated due to the shape mixing. In order to improve upon the theory of fission, we shall consider the inclusion of several collective coordinates and the dynamics of spontaneous fission process, the improved energy density functionals [12], and the full ATDHFB inertia parameters. The work is in progress. Some introductory results will be published soon [13].

This work was supported in part by the National Science Center (Poland) under Contract DEC-2011/01/B/ST2/03667.

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