MASSES OF HEAVIEST DEFORMED NUCLIDES

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Masses of the heaviest deformed even–even nuclides with the atomic number Z = 98–114 have been calculated by applying a macroscopic–microscopic method. Approximate formulas for calculating masses of odd and odd–odd nuclides from the calculated masses of the neighboring even–even nuclides and the average pairing energies of unpaired nucleons are used. For the 56 heaviest deformed nuclides, for which masses are experimentally known, the standard deviation of 0.30 MeV has been obtained.

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1. Introduction

Since the mid 1970-ties, when the reactions based on ^{208}Pb and ^{209}Bi targets have been proposed to produce the heaviest atomic nuclei [1], great progress has been made in discovering deformed superheavy nuclei. Elements with atomic numbers Z = 107–112 have been synthesized and their alpha-decay descendants have been produced [2]. The confirmation experiments have been performed [3, 4]. Moreover, a number of odd element isotopes has been produced in a combination with ^{208}Pb targets and odd element projectiles [5, 6]. The synthesis of element 113 has also been reported [7]. However, so far only masses of 56 nuclides with the atomic number $Z = 98$–110 are experimentally known [8].

The objective of the present paper is to present the macroscopic–microscopic calculation of masses of the deformed even–even nuclides with $Z =$ 98–114. The region of nuclides chosen for the calculation is limited by extremely small formation cross sections and the neighboring region of spherical superheavy nuclides. Moreover, we use straightforward formulas for calculating masses of odd and odd–odd nuclides from the calculated masses of the neighboring even–even nuclides and the average pairing energies of unpaired nucleons. Earlier, we applied the same model for calculating masses of the hypothetical at that time spherical superheavy nuclides [9]. Recently, the synthesis of spherical superheavy nuclei with atomic numbers up to $Z = 118$ in reactions with actinide targets and ^{48}Ca projectile and the production of their alpha-decay descendants has been reported [10]. A number of these nuclides has been obtained in later independent experiments [11–16]. Mass of none spherical superheavy nuclide is experimentally known.

It is worth mentioning that, with the use of the same model as the model applied in the present paper, the equilibrium deformation of the heaviest deformed even–even nuclei has been calculated in Ref. [17]. For the vast majority of the considered nuclei the main quadrupole component of deformation $\beta_2 = 0.20$–0.25 has been obtained. That prediction is consistent with the later measurement of quadrupole deformation of ^{254}No [18].

The contribution of an unpaired nucleon to the mass of a nucleus may be treated in one of three ways. The most complicated and usually disregarded for heaviest nuclides way consists in blocking for pairing interaction a single-particle nuclear state for which the nuclear energy is minimal. In this method, one chooses a blocked state among the several ones above and the several ones below the Fermi level. This action is repeated in each step of the minimization of nuclear energy with respect to deformation. The second method consists in adding a lowest quasiparticle energy of an unpaired nucleon to the ground-state mass of a nucleus. In the third method, which is the simplest and with the accuracy not smaller than the previous two methods, one adds the average pairing energy of a nucleon to the ground-state mass of a nucleus. The latter we obtained as the arithmetic average of masses of the neighboring even–even nuclei. In the present study, the third method is used.

In the macroscopic–microscopic calculations of masses of deformed nuclides described in Refs. [19, 20] the authors added to the mass formula the zero-point vibration energy in a rough parabolic approximation different for each nucleus. In Ref. [19], the authors considered even–even nuclei, used the three-dimensional deformation space and the BCS pairing approach with introduced a new pairing strength. Their refitted values of the macroscopic parameters are the following: $\kappa_{\rm V} = 1.962$ and $c_{\rm a} = 0.330$ MeV. The authors of Ref. [20] considered even–even and odd nuclei, used the four-dimensional deformation space and the Lipkin–Nogami pairing approach with a pairing strength taken from Ref. [21]. The contribution of an odd nucleon to the ground state mass of a nucleus they described by adding its lowest quasiparticle energy. Their refitted values of the macroscopic parameters read $\kappa_{\rm V} = 1.92552$ and $c_{\rm a} = 0.14505$ MeV. In Ref. [22] even–even, odd and odd–odd nuclei have been considered. The BCS pairing approach has been used with the pairing strength taken from Ref. [23]. To describe the contribution of an odd nucleon to the ground state mass of a nucleus its lowest quasiparticle energy was added. The macroscopic energy has been calculated without the Wigner term and the charge-asymmetry term $c_{\rm a}(N-Z)$, where N is the neutron number and Z is the atomic number. The refitted macroscopic parameters are $a_{\rm V} = 16.0643$ MeV, $\kappa_{\rm V} = 1.9261$ and $a_0 = 17.926$ MeV. In the calculation of nuclear masses, seven dimensional deformation space has been applied. In Ref. [24], the same model as in Ref. [22] has been used to calculate the nuclear masses, as well as the fission barriers, for the wider region of even–even nuclides ranging up to $Z = 126$, also for neutron deficient nuclides far behind the reach of the present-day experiments. From both studies [22, 24], one can draw a conclusion that the odd-multipolarity deformations are equal to zero for deformed superheavy nuclei reducing the deformation space for these nuclei to four dimensions. In our calculation described in the present paper, we consider even–even, odd and odd–odd nuclides. We use the BCS pairing approach with the pairing strength from Ref. [19]. We describe the contribution of an odd nucleon adding the average pairing energy to the ground state of a nucleus. We use the four-dimensional deformation space. Our refitted macroscopic parameters read $\kappa_{\rm V} = 1.990$, $c_{\rm a} = 0.572$ MeV and $a_0 = 13.8$ MeV. In the above discussed calculations, the Woods–Saxon potential was used to obtain the single-particle energy spectra necessary to calculate the microscopic energy and a restricted region of nuclei from ^{208}Pb upward was used to refit some of the macroscopic parameters. Differences between the models discussed above are collected in Table I.

Our calculation, mainly due to the use of a smaller region of nuclei to determine the macroscopic parameters, as well as the use of a larger deformation space, the Woods–Saxon potential and carefully chosen description of pairing, gives pretty small standard deviation. In other words, the above mentioned features of our calculation lead to increased predictive power. We obtained standard deviation of 0.35 MeV, smaller than 0.37 MeV obtained in Ref. [22] for nuclei heavier than ^{208}Pb, and significantly smaller than about half MeV obtained in FRLDM and FRDM models [25] for these nuclei. In the latter two models, besides the fit of macroscopic parameters to nuclei from ^{16}O upward and the use of the smaller three-dimensional deformation space, the Yukawa potential was applied to obtain the single-particle spectra for neutrons and protons used for calculating the microscopic energy.

2. The model and the results

In the calculation of masses of the even–even nuclides, we applied a macroscopic–microscopic model. We calculated the microscopic part of nuclear energy originating from the shell effects using the Strutinski method [26]. In order to apply it, we calculated the single-particle energy levels solving the Schrödinger equation separately for neutrons and protons.

TABLE I

Ingredients of the macroscopic–microscopic models in which restricted range of nuclei in fitting macroscopic parameters has been used.

Reference	Nuclei considered	Number of shape parameters	The zero-point energies	Pairing approach	Pairing strength	Pairing energy of an unpaired nucleon	Macroscopic terms omitted	Macroscopic parameters refitted
[19]	even–even	3	yes	BCS	[19]	N/A	none	$\kappa_{\rm V} = 1.962$ $c_{\rm a} = 0.330$ MeV
[20]	even–even odd	4	yes	Lipkin–Nogami	[21]	lowest quasiparticle energy	none	$\kappa_{\rm V} = 1.92552$ $c_{\rm a} = 0.14505$ MeV
[22]	even–even odd odd–odd	4	no	BCS	[23]	lowest quasiparticle energy	Wigner term charge-asymmetry energy	$a_{\rm V} = 16.0643$ MeV $\kappa_{\rm V} = 1.9261$ $a_0 = 17.926$ MeV
[24]	even–even	4	no	BCS	[23]	lowest quasiparticle energy	Wigner term charge-asymmetry energy	$a_{\rm V} = 16.0643$ MeV $\kappa_{\rm V} = 1.9261$ $a_0 = 17.926$ MeV
Present paper	even–even odd odd–odd	4	no	BCS	[19]	average pairing energy	none	$\kappa_{\rm V} = 1.990$ $c_{\rm a} = 0.572$ MeV $a_0 = 13.8$ MeV

The Woods–Saxon single-particle Hamiltonian [27] with the universal parameters [27] we diagonalized in the axially deformed harmonic oscillator basis [27]. We used the basis with 19 harmonic oscillator shells for both neutrons and protons with 550 lowest laying neutron and 350 lowest lying proton states. To describe the pairing interaction, we used the BCS approach. We calculated the pairing correction, which is a part of the microscopic energy, using the strength of pairing taken from Ref. [19]. It is worth noting that the pairing correction originating from many quasiparticle states should not be confused with the average pairing energy of an unpaired nucleon.

We used the Yukawa-plus-exponential formula [28] as the macroscopic energy. We parametrized nuclear shapes through the spherical harmonics. We checked out in Ref. [29] that for calculating masses of the heaviest deformed nuclides the nuclear energy should be minimalized in the four-dimensional deformation space $\{\beta_2, \beta_4, \beta_6, \beta_8\}$ describing axially symmetric shapes. This is because the deformation β_8 decreases masses by about half MeV and the deformation β_{10} leaves masses practically unchanged. The readjustment of parameters in the macroscopic part of the mass formula was done to 77 experimentally known masses [30] of even–even nuclides laying on the nuclear chart above the proton shell 82 and the neutron shell 126, as well as to those with $Z = 82$ and $N = 126$, to obtain a smaller standard deviation of the results for the superheavy nuclides. In other words, to obtain better predictive power of calculated masses of the heaviest nuclides. The parameters in terms dependent on deformation have not been refitted in order not to spoil the values of the fission barriers [17] and, consequently, the values of the spontaneous-fission half-lives [17]. The refitted parameters read [31]: the volume-asymmetry parameter $\kappa_{\mathrm{V}} = 1.990$, the charge-asymmetry parameter $c_{\mathrm{a}} = 0.572$ MeV and the constant $a_0 = 13.8$ MeV. The obtained standard deviation for the even–even nuclei with $Z \geq 82$ and $N \geq 126$ is equal to 0.26 MeV.

Approximate formulas for masses, in MeV, of the heaviest odd nuclides may be given adding the average pairing energy of an unpaired nucleon 12 MeV$/\sqrt{A}$ [32] to the arithmetic average of the calculated masses of the neighboring even–even nuclides. A formula for an odd-N nuclide is the following

$$M(Z,N) = \tfrac{1}{2}[M(Z,N-1) + M(Z,N+1)] + \frac{12\ \mathrm{MeV}}{\sqrt{A}}\,, \tag{1}$$

where $M(Z,N)$ is the mass of a nuclide with the atomic number Z, the neutron number N and the mass number $A = Z + N$. Similarly, a formula for an odd-Z nuclide is the following

$$M(Z,N) = \tfrac{1}{2}[M(Z-1,N) + M(Z+1,N)] + \frac{12\ \mathrm{MeV}}{\sqrt{A}}\,. \tag{2}$$

Approximate formula for mass, in MeV, of the heavy odd–odd nuclide may be given adding the sum of the average pairing energy of an unpaired proton and an unpaired neutron to the arithmetic average of the calculated masses of the neighboring even–even nuclides. For an odd-N and odd-Z nuclide a formula reads

$$M(Z,N) = \tfrac{1}{4}[M(Z-1,N-1)+M(Z+1,N-1)+M(Z-1,N+1) + M(Z+1,N+1)] + \frac{24\ \mathrm{MeV}}{\sqrt{A}}\,. \quad (3)$$

In Table II, there is collected the calculated mass of the deformed even–even nuclides with $Z = 98$–114 as the mass excess, *i.e.*, $[M(\mathrm{in}\ u) - A]$, in MeV, where M is the mass of a nuclide, u is the atomic mass unit and A is the mass number. The region of nuclides chosen for the calculation is limited by extremely small formation cross sections and the neighboring region

TABLE II

Calculated mass excess, in MeV, of the heaviest deformed even–even nuclides with the atomic number $Z = 98$–114 and the neutron number N given in the first column.

N	Cf	Fm	No	Rf	Sg	Hs	Ds	Cn	114
132	61.92								
134	60.07	74.48							
136	58.81	72.36	87.64						
138	58.16	70.80	85.20	101.35					
140	58.09	69.79	83.32	98.63	115.58				
142	58.63	69.39	82.02	96.48	112.59	130.45			
144	59.81	69.59	81.35	94.93	110.18	127.19	146.06		
146	61.67	70.46	81.30	93.98	108.33	124.46	142.54	162.26	
148	64.21	72.01	81.87	93.57	106.98	122.25	139.54	158.50	178.98
150	67.37	74.14	82.99	93.72	106.18	120.59	137.08	155.28	175.01
152	71.11	76.90	84.73	94.51	106.05	119.58	135.28	152.72	171.70
154	75.78	80.68	87.59	96.36	106.90	119.49	134.39	151.03	169.18
156	81.08	85.11	91.07	98.85	108.39	120.02	134.09	149.88	167.19
158	86.76	89.94	94.96	101.76	110.34	121.01	134.21	149.11	165.56
160	92.80	95.11	99.23	105.08	112.73	122.41	134.68	148.70	164.29
162	99.11	100.60	103.83	108.80	115.55	124.28	135.64	148.77	163.54
164		107.20	109.68	113.90	119.88	127.77	138.10	150.19	163.95
166			116.01	119.50	124.79	131.89	141.23	152.36	165.16
168				125.49	130.04	136.43	144.83	155.01	166.91
170					135.54	141.24	148.70	157.90	168.95
172						145.95	152.52	160.93	171.17
174							156.71	164.29	173.67

of spherical superheavy nuclides. We obtained standard deviation equal to 0.30 MeV for 56 heaviest nuclides for which masses are experimentally known. The differences between the calculated masses in the present paper and experimentally known masses [8] of the even–even, odd and odd–odd heaviest deformed nuclides are collected in Table III.

TABLE III

Differences, in MeV, between the calculated masses in the present paper and the experimentally known masses [8] of even–even, odd and odd–odd heaviest deformed nuclides with the atomic number $Z = 98$–110. The neutron number N is given in the first column.

N	Cf	Es	Fm	Md	No	Lr	Rf	Db	Sg	Bh	Hs	Mt	Ds
139	0.97												
140													
141													
142	0.64												
143													
144	0.42												
145													
146	0.19		0.27										
147	0.32												
148	0.12	0.29	0.11										
149	0.45		0.31										
150	0.13		0.07	0.35	0.11								
151	0.27		0.32		0.26								
152	−0.06	0.25	0.08		0.01	0.42	0.29						
153	0.06	0.33	0.19		0.10	0.55	0.32						
154	−0.26	−0.04	−0.22	0.04	−0.23		0.02	0.39	0.36				
155	−0.12	0.18	−0.15		−0.17				0.38				
156	−0.26	−0.24	−0.38	−0.16					0.02		0.44		
157			−0.31	0.07			−0.27				0.35		
158											−0.14		
159													0.33
160													0

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