Structure of Odd-*N* Superheavy Elements

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Structure of the odd-N superheavy elements with $Z \lesssim 118$ and $N \lesssim 175$ is investigated using the self-consistent Skyrme-Hartree-Fock-Bogoliubov method with pairing. Microscopic analysis of one-quasiparticle neutron states, alpha-decay energies, and deformations is performed. Good agreement was obtained with the recently reported α-decay chains of $^{289}114$ and $^{293}118$.

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One of the fundamental and persistent questions of nuclear science concerns the maximum charge and weight that the nucleus may attain. Amazingly, even after thirty-or-so years of our quest for the superheavy elements, the borders of the upper-right end of the nuclear chart are unknown. Theoretically, the mere existence of the heaviest elements with $Z \gtrsim 104$ is entirely due to quantal shell effects. Indeed, for these nuclei the classical nuclear droplet, governed by surface tension and Coulomb repulsion, fissions immediately due to the huge electric charge. At the end of the sixties, a number of theoretical predictions were made that pointed towards the existence of long-lived superheavy (SHE) nuclei [1–5]. However, it is only during recent years that significant progress in the production of the heaviest nuclei has been achieved [6,7]. Notably, three new elements, $Z = 110$, 111, and 112, were synthesized by means of both cold and hot fusion reactions [8–10]. These heaviest isotopes decay predominantly by groups of α particles (α chains) as expected theoretically [11–13].

All the heaviest elements found recently are believed to be well deformed. Indeed, the measured α-decay energies, along with complementary syntheses of new neutron-rich isotopes of elements $Z = 106$ and $Z = 108$, have furnished confirmation of the special stability of the deformed shell at $N = 162$ predicted by theory [14,15]. Still heavier and more neutron-rich elements are expected to be spherical and even more strongly stabilized by shell effects.

There is no consensus among theorists with regard to the center of the shell stability in the region of spherical SHE. For the neutrons, most calculations predict a magic gap at $N = 184$. However, because of different treatments of the large Coulomb potential and spin-orbit interaction, various models yield different predictions for the position of the magic proton gap (cf. discussion in Ref. [16]). While $Z = 114$ was predicted to be the next magic proton number in the macroscopic-microscopic models [11,15], the recent self-consistent models [16,17] favor spherical shell closures at $Z = 126$, 124, and 120. In this context, the synthesis of the $N = 175$ isotones reported by the Dubna and Livermore (DL) Collaboration ($Z = 114$) [18] and the Berkeley and Oregon (BO) team ($Z = 118$) [19] is both exciting and important. In both cases, the evidence is based on the observed α-decay chains (one in the DL experiment and three in the BO experiment). Because of the large neutron number of the compound nucleus, these α chains do not terminate at some known systems. Consequently, until the charge-mass identification is made, one can use theoretical arguments to support/disprove the experimental assignment. This is the subject of this Letter.

Recently, we have performed a large-scale self-consistent study of properties of even-even, A-odd, and odd-odd heaviest nuclei. Detailed results of this work will be published elsewhere [20]. Here, we present the small subset of our results relevant to the DL and BO experiments. In our work, we have used the Hartree-Fock-Bogoliubov (HFB) method with a Skyrme interaction in the particle-hole (p-h) channel and a delta force in the pairing channel. The details of calculations closely follow Ref. [16]. The HFB equations have been solved in the coordinate space according to the method of Ref. [21]. The actual mesh is very dense; it consists of 17^3 points with a mesh step of 0.8 fm. This has allowed a very accurate determination of binding energies. In the p-h channel, the Skyrme effective interaction SLy4 has been used. This parametrization [22] has been, in particular, adjusted to reproduce long isotopic sequences; hence one can expect it to have good isospin properties. In order to minimize unphysical fluctuations of the pairing field in regions of low level density, an approximate particle number projection was implemented by means of the Lipkin-Nogami method [23,24]. The pairing strengths of the interaction have then been adjusted to reproduce the average proton and neutron pairing gaps in even-even nuclei around ^{254}Fm. The properties of one-quasiparticle states were calculated by means of the self-consistent blocking. In addition, the odd-T terms that appear in the intrinsic Hamiltonian due to nonzero spin [25] were

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properly considered. To the best of our knowledge, this work is the first self-consistent study of one-quasiparticle states in SHE that properly treats the polarization due to the odd (unpaired) particle.

Any theoretical model aiming at making predictions in an unknown territory should first be tested in known regions of the chart of the nuclides. Since the main decay mode for the known heaviest elements is α decay, one of the crucial quantities determining lifetimes of the heaviest and superheavy elements is the α-decay energy. The Q_α values for the heaviest elements calculated with the HFB-SLy4 model are displayed in Fig. 1. They are compared with known α-decay energies. It is seen that the agreement with experimental data is very good. The only deviation is for the $N = 152$ isotones of Cm, Cf, and Fm, where calculations overestimate the experimental values of Q_α by $\sim$500 keV. (This is due to the $N = 152$ deformed shell closure which is slightly underestimated by theory.) The good agreement with experimental data that we obtain convinces us that the HFB-SLy4 model can be used to predict properties of unknown SHE.

In order to gain some understanding about the single-particle shell structure around ^{284}112, we show in Fig. 2 the predicted proton and neutron levels along the α chain of even-even nuclei starting at ^{260}Fm and ending at ^{296}118. The ground-state (g.s.) mass quadrupole deformation β_2 (defined according to Ref. [16]) decreases along this chain from the value of $\beta_2 \approx 0.26$ at the deformed subshell closure at $N = 162$ to $\beta_2 \approx 0$ when approaching the magic gap $N = 184$ [16]. Around $N = 174$, quadrupole deformation takes intermediate values, $\beta_2 \approx 0.13$.

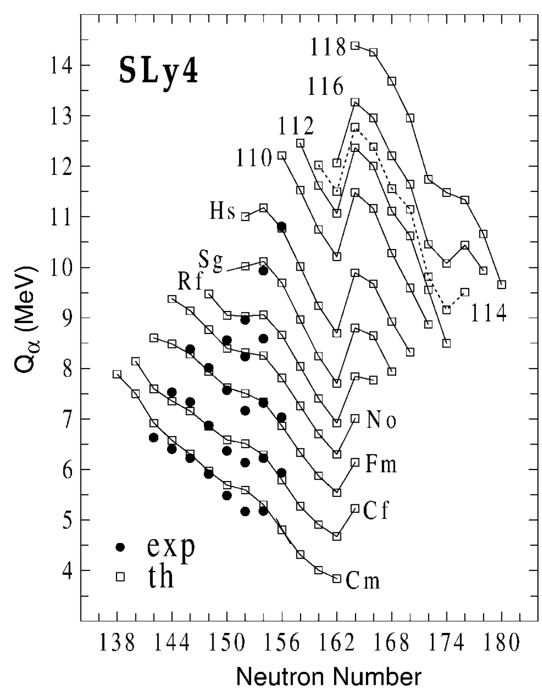

FIG. 1. Q_α values for even-even nuclei with $96 \leq Z \leq 118$ obtained in the HFB-SLy4 model. The experimental Q_α values (filled circles) are taken from Refs. [7,26].

As far as the protons are concerned, no significant shell effects are seen between the well-known deformed gap at $Z = 108$ and that at $Z = 118$, which appears at higher neutron numbers and smaller deformations. In particular, in the region of particle numbers considered, *no* shell effect at $Z = 114$ is present. On the other hand, there appears a very interesting shell structure in the neutron system. For the nuclei with $Z > 110$ the 175th neutron occupies the isolated Nilsson orbital $[707]\frac{15}{2}^-$ originating from the $1j_{15/2}$ shell. This level separates the large single-particle gaps at $N = 174$ and 176. For nuclei with $164 < N < 174$, there are several single-neutron levels around the Fermi level, namely the positive-parity orbitals $[611]\frac{1}{2}^+$, $[606]\frac{11}{2}^+$, $[604]\frac{9}{2}^+$, $[611]\frac{3}{2}^+$, and $[613]\frac{5}{2}^+$, and the

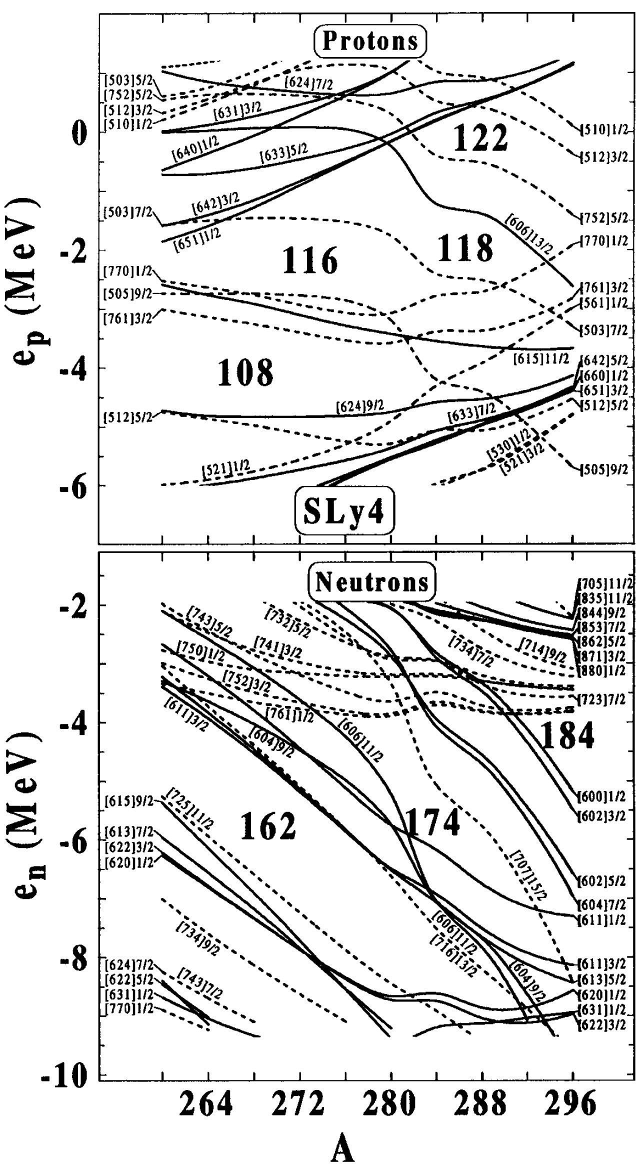

FIG. 2. Proton (top) and neutron (bottom) single-particle levels calculated in the HFB-SLy4 model for the α chain of even-even nuclei: $(Z,N) = (100,160)$, $(102,162), \ldots,$ $(118,178)$. Note that in the self-consistent method each of these nuclei has different ground-state deformations.

negative-parity level $[716]\frac{13}{2}^-$. As discussed below, the level bunching below $N = 174$ and the presence of the high-Ω orbital at $N = 175$ has significant consequences for the α-decay properties of $^{289}114$ and $^{293}118$.

The calculated one-quasiparticle structures and the g.s.-to-g.s. values of Q_α in the $^{289}114$ and $^{293}118$ α-decay chains are shown in Tables I and II, respectively. Using this data, other Q_α values for all the low-lying states shown in Tables I and II can easily be obtained. For instance, for the α transition between the excited $[611]\frac{1}{2}^+$ level in $^{289}114$ and the $[611]\frac{1}{2}^+$ g.s. of $^{285}112$ $Q_\alpha = 9.64$ MeV + 0.52 MeV = 10.16 MeV.

According to our calculations, the g.s-to-g.s. α decays of $^{289}114$ and $^{293}118$ are structurally forbidden since the g.s. properties of parent and daughter nuclei differ dramatically. The allowed transitions to the excited $[707]\frac{15}{2}^-$ level in $^{285}112$ and $^{289}116$ correspond to $Q_\alpha = 9.0$ MeV and $Q_\alpha = 10.9$ MeV, respectively, and are considerably lower than the experimental values (DL: 9.9 MeV; BO: 12.6 MeV). Consequently, the most probable candidates for the first α transitions are the 10.2 MeV ($^{289}114$) and 11.8 MeV ($^{293}118$) lines associated with the allowed $[611]\frac{1}{2}^+ \rightarrow [611]\frac{1}{2}^+$ decays. By the same token, the $[611]\frac{1}{2}^+$ g.s. of $N = 173$ isotones is expected to decay to the excited $[611]\frac{1}{2}^+$ level in the $N = 171$ daughters. For $^{285}112$, the corresponding Q_α energy, 8.76 MeV, is very close to the experimental energy of the second α transition, 8.84 MeV, reported by the DL group. For the $^{289}116$ decay we obtain $Q_\alpha = 10.14$ MeV, i.e., we underestimate the energy of the second α particle (11.8 MeV) from the BO experiment. This is the worst deviation from experiment obtained in our calculations.

The $[611]\frac{1}{2}^+$ level is also expected to be the ground state of the $N = 169$ isotones, and our prediction for the allowed $[611]\frac{1}{2}^+ \rightarrow [611]\frac{1}{2}^+$ decays is 9.4 MeV for $^{281}110$ and 10.6 MeV for $^{285}114$. Again, we obtain excellent agreement with the DL data (9.0 MeV) and underestimate the energy of the third α transition in the BO experiment (11.5 MeV).

For the α transitions in the $^{281}112 \rightarrow \cdots \rightarrow {}^{265}104$ chain, allowing the positive-parity Nilsson orbitals with very similar quantum numbers, we obtain the following values of Q_α: 10.7 MeV (BO: 10.8 MeV), 11.1 MeV (BO: 10.3 MeV), 9.9 MeV (BO: 9.9 MeV), 8.0–8.5 MeV (BO: 8.9 MeV). An alternative route is possible that involves α transitions between $j_{15/2}$ orbitals. Here, for the last two Q_α values we obtain 9.8 and 8.7 MeV. In both cases we obtain good agreement with BO data. Table I also shows the predicted structure of $^{293}116$. The g.s. of this transitional nucleus ($\beta_2 \approx 0.09$) is a $[604]\frac{7}{2}^+$ Nilsson level. The Q_α value for the allowed α decay to the excited $[604]\frac{7}{2}^+$ state in $^{114}289$ is 9.7 MeV.

According to Ref. [18], the maximum cross section for producing evaporation residues in the DL experiment corresponds to the $3n$-evaporation channel but the $2n$ ($^{290}114$) and $4n$ ($^{288}114$) channels cannot be excluded. The Q_α values calculated for the g.s. → g.s. α-decay chains of $^{290}114$ and $^{288}114$ are 9.7, 8.5, 8.9 MeV and 9.4, 9.4, 9.8 MeV, respectively. It is seen, therefore, that the experimental data are also consistent with the α-decay chain of $^{290}114$. On the other hand, for the α evaporation channel in the BO experiment [19] (the $^{290}116$ α chain) our calculations yield 10.2, 9.6, 10.8, 10.6, 9.9, 9.0, 6.9 MeV; i.e., the agreement is considerably worse compared to the $^{293}118$ scenario.

In summary, we present the first self-consistent analysis of one-quasineutron states in SHE. The calculated equilibrium deformations of one-quasiparticle states in $N = 175$ isotones are rather small ($\beta_2 \approx 0.11$), and they increase along the α-decay chain. This trend reflects the influence of the $N = 184$ magic neutron gap for the heaviest systems and the deformed $N = 162$ gap for the

TABLE I. Predicted structure of the lowest one-quasi-particle excitations in the $^{293}116$ α-decay chain. Each excitation is characterized by the Nilsson quantum numbers of the odd neutron, excitation energy, and quadrupole deformation. The number in parentheses indicates the Q_α value for the ground-state to ground-state transition.

Nucleus	Orbital	Energy (MeV)	β_2
$^{293}116$	$[604]\frac{7}{2}^+$	0	0.09
(10.47)	$[602]\frac{5}{2}^+$	0.31	0.09
	$[611]\frac{1}{2}^+$	0.52	0.08
	$[707]\frac{15}{2}^-$	0.93	0.09
$^{289}114$	$[707]\frac{15}{2}^-$	0	0.12
(9.64)	$[611]\frac{1}{2}^+$	0.52	0.11
	$[604]\frac{7}{2}^+$	0.79	0.13
	$[602]\frac{5}{2}^+$	1.17	0.12
$^{285}112$	$[611]\frac{1}{2}^+$	0	0.14
(8.88)	$[611]\frac{3}{2}^+$	0.60	0.14
	$[707]\frac{15}{2}^-$	0.62	0.13
	$[606]\frac{11}{2}^+$	0.65	0.15
	$[604]\frac{9}{2}^+$	0.72	0.15
$^{281}110$	$[604]\frac{9}{2}^+$	0	0.19
(9.32)	$[606]\frac{11}{2}^+$	0.07	0.19
	$[611]\frac{1}{2}^+$	0.12	0.18
	$[611]\frac{3}{2}^+$	0.59	0.17
	$[613]\frac{5}{2}^+$	0.65	0.17
	$[716]\frac{13}{2}^-$	0.94	0.17
$^{277}108$	$[611]\frac{1}{2}^+$	0	0.21
	$[604]\frac{9}{2}^+$	0.04	0.20
	$[613]\frac{5}{2}^+$	0.31	0.21
	$[716]\frac{13}{2}^-$	0.36	0.21
	$[611]\frac{3}{2}^+$	0.38	0.20

TABLE II. Same as in Table I, except for the $^{293}118$ α-decay chain.

Nucleus	Orbital	Energy (MeV)	β_2
$^{293}118$	$[707]\,\frac{15}{2}^-$	0	0.11
(11.59)	$[611]\,\frac{1}{2}^+$	0.16	0.10
	$[602]\,\frac{5}{2}^+$	0.84	0.12
	$[604]\,\frac{7}{2}^+$	0.98	0.10
$^{289}116$	$[611]\,\frac{1}{2}^+$	0	0.13
(10.18)	$[606]\,\frac{11}{2}^+$	0.62	0.14
	$[611]\,\frac{3}{2}^+$	0.66	0.13
	$[604]\,\frac{9}{2}^+$	0.69	0.14
	$[707]\,\frac{15}{2}^-$	0.72	0.13
$^{285}114$	$[606]\,\frac{11}{2}^+$	0	0.16
(10.60)	$[611]\,\frac{1}{2}^+$	0.04	0.16
	$[611]\,\frac{3}{2}^+$	0.15	0.16
	$[604]\,\frac{9}{2}^+$	0.16	0.16
	$[613]\,\frac{5}{2}^+$	0.28	0.15
	$[716]\,\frac{13}{2}^-$	0.73	0.16
$^{281}112$	$[611]\,\frac{1}{2}^+$	0	0.19
(10.85)	$[604]\,\frac{9}{2}^+$	0.07	0.19
	$[611]\,\frac{3}{2}^+$	0.37	0.19
	$[613]\,\frac{5}{2}^+$	0.41	0.19
	$[606]\,\frac{11}{2}^+$	0.42	0.19
	$[716]\,\frac{13}{2}^-$	0.51	0.19
$^{277}110$	$[716]\,\frac{13}{2}^-$	0	0.22
(11.07)	$[613]\,\frac{5}{2}^+$	0.02	0.21
	$[611]\,\frac{3}{2}^+$	0.07	0.21
	$[611]\,\frac{1}{2}^+$	0.15	0.22
	$[604]\,\frac{9}{2}^+$	0.27	0.21
	$[606]\,\frac{11}{2}^+$	0.83	0.21
$^{273}108$	$[611]\,\frac{3}{2}^+$	0	0.23
(9.93)	$[613]\,\frac{5}{2}^+$	0.04	0.23
	$[716]\,\frac{13}{2}^-$	0.05	0.23
	$[604]\,\frac{9}{2}^+$	0.54	0.22
	$[611]\,\frac{1}{2}^+$	0.55	0.23
$^{269}106$	$[611]\,\frac{3}{2}^+$	0	0.24
(8.45)	$[613]\,\frac{5}{2}^+$	0.15	0.24
	$[716]\,\frac{13}{2}^-$	0.22	0.22
	$[604]\,\frac{9}{2}^+$	0.60	0.24
$^{265}104$	$[725]\,\frac{11}{2}^-$	0	0.25
	$[604]\,\frac{9}{2}^+$	0.09	0.25
	$[613]\,\frac{7}{2}^+$	0.42	0.25
	$[622]\,\frac{3}{2}^+$	0.79	0.25

lightest nuclei in the chain. As far as Q_α values, our calculations are consistent with the recent experimental findings of Refs. [18] and [19]. In particular, the DL data can be interpreted in terms of the α chains of $^{289}114$ or $^{290}114$. We also obtain good agreement with the BO data assuming the $^{293}118$ α chain. The ground state of the $N = 175$ isotones is calculated to be a high-Ω *isomeric* state $[707]\,\frac{15}{2}^-$. Because of structural arguments, this state is probably bypassed. (The same is true for the high-Ω ground state of $N = 171$.) This result may explain the observed lower cross section for the production of $^{293}118$ ($\sim$2 pb) as compared to calculations by Smolańczuk [13] ($\sim$670 pb).

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