Candidates for long-lived high-K ground states in superheavy nuclei

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On the basis of systematic calculations for 1364 heavy and superheavy (SH) nuclei, including odd systems, we have found a few candidates for high-K ground states in superheavy nuclei. The macroscopic-microscopic model based on the deformed Woods-Saxon single-particle potential that we use offers a reasonable description of SH systems, including known nuclear masses, Q_α values, fission barriers, ground state (g.s.) deformations, and super- and hyperdeformed minima in the heaviest nuclei. Exceptionally untypical high-K intruder contents of the g.s. found for some nuclei, accompanied by a sizable excitation of the parent configuration in the daughter, suggest a dramatic hindrance of the α decay. Multidimensional hypercube configuration-constrained calculations of the potential energy surfaces (PESs) for one especially promising candidate, ^{272}Mt, shows a $\simeq 6$ MeV increase in the fission barrier above the configuration-unconstrained barrier. There is a possibility that one such high-K ground or low-lying state may be the longest-lived superheavy isotope.

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I. INTRODUCTION

Two current methods of making superheavy elements in the laboratory, cold [1,2,3] and hot [4] fusion reactions, seem to have reached their limits. In the first one, (i) evaporation residues (ERs) produced on Pb or Bi targets are far from the predicted island of stability, and (ii) ER cross sections drop steeply with the mass of a projectile. In the latter, with the ^{48}Ca projectile impinging on various actinide targets, ER cross sections are roughly constant. However, once the element $Z = 118$ has been synthesized [5], attempts to go beyond hit two obstacles: (i) a difficulty or impossibility of making targets from Es and heavier actinides, and (ii) reactions with heavier projectiles such as ^{50}Ti, ^{54}Cr, ^{58}Fe, and ^{64}Ni have not produced any ERs up to now.

On the other hand, not all superheavy (SH) isotopes $Z \leqslant 118$ have been produced yet. It might be that among them hides some surprisingly long-lived one, either in its ground or excited isomeric state. It is even not excluded that such a long-lived SH state was already produced, but remained undetected. Since detection procedures used at present are adjusted to short-time coincidences, a species living tens of minutes would be very likely missed in the background. Therefore, while pondering possible new reactions leading towards the island of stability, it may be worthwhile to search for long-lived exotic SH configurations. Obvious candidates are high-K isomers or groundstates, for which increased stability is expected due to some specific hindrance mechanisms. The present paper provides predictions and arguments for such long-lived SH states.

The existence of isomeric states is rather well established in nuclear structure physics [6]. The structure of expected long-lived multiquasiparticle high-spin isomers in some even-even SH nuclei was analyzed, e.g., in [7]. In particular, the assignments of 9^- or 10^- [8] two-quasineutron configurations for the $6.0^{+8.2}_{-2.2}$ ms isomer in ^{270}Ds (the heaviest isomer known) was supported [7]. Let us stress that the half-life of this isomer is much longer than that of the ground state (100^{+140}_{-40} μs). The same holds for the 8^+ isomer in ^{256}Es, with a half-life of 7.6 h; significantly longer than the 25 min of the ground state (g.s.). Another interesting example is a 16^+ or 14^+ state in ^{254}No, with a half-life of 184 μs, at 2.93 MeV above g.s. [9–13]. In [14], the four-quasiparticle isomers around ^{254}No were postulated. All examples described above relate to prolate equilibria. A possibility of high-K isomers at the superdeformed oblate minima in SH nuclei was indicated in [15].

The electromagnetic stability of an isomeric state is difficult to predict as it depends on fine details of the single particle (s.p.) structure. Therefore, we concentrate here on high-K ground states or very-low-lying configurations in odd-A and odd-odd nuclei. Excited configurations are also of interest, as some detected α transitions, and even whole portions of α decay chains, may actually connect not g.s., but excited states of similar structure. The hindrance of the spontaneous fission (s.f.) in odd-odd relative to even-even isotopes by several orders of magnitude is well established in heavy nuclei. It is also known from experimental studies that α decays accompanied by a change of the parent configuration are hindered with respect to configuration-preserving transitions. It is understood as a decrease in the probability of the α-particle formation when different parent and daughter configurations are involved. The α-decay rate shows also the exponential dependence on the barrier between the α particle and the daughter nucleus. When a parent configuration has some excitation energy in the daughter, this barrier increases and an effective Q_α value decreases by this energy. If the configuration-changing decays had been hindered completely, the α-decay rate would have been given by the reduced Q_α

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values. In reality, a degree of the configuration hindrance is surely configuration dependent.

II. METHOD OF CALCULATION

In order to predict possible exotic configurations one has to have a reliable model to find ground states in odd and odd-odd nuclei. We used the macroscopic-microscopic model based on a deformed Woods-Saxon potential [16] and the Yukawa plus exponential macroscopic energy [17] Recently, within this approach (with parameters adjusted to heavy nuclei [18]), it was possible to reasonably reproduce data on first [19], second [20,21], and third [22,23] fission barriers and systematically predict ground states and saddle points in even-even superheavy nuclei up to $Z = 126$ [24].

For systems with an odd numbers of protons or neutrons (or both), we used a standard blocking method. The ground states were found by minimizing over configurations (blocking particles on levels from the 10th below to 10th above the Fermi level) and deformations. For nuclear ground states it was possible to confine analysis to axially-symmetric shapes. In the present study, four mass- and axially-symmetric deformations, β_{20}, β_{40}, β_{60}, and β_{80}, were used; see [25]. Minimization is performed by the gradient method and on the mesh of deformations; see [25]. Both sets of results are consistent. As an additional check, we performed another set of calculations of nuclear masses within the quasiparticle method. These calculations are much simpler and we were able to perform a seven-dimensional minimization over axially-symmetric deformations β_{20}, β_{30}, β_{40}, β_{50}, β_{60}, β_{70}, and β_{80}.

A simplest extension of the Woods-Saxon (WS) model to odd nuclei required three new constants which may be interpreted as the mean pairing energies for even-odd, odd-even, and odd-odd nuclei [25]. They were fixed by a fit to the masses with $Z \geqslant 82$ and $N > 126$ via minimizing the rms deviation in particular groups of nuclei, which is a rather standard procedure [26,27]. Masses of nuclei were taken from [28]. The obtained rms deviation in masses for 252 nuclei was about 400 keV with blocking and around 300 keV with the quasiparticle method. Similar rms errors resulted for 204 Q_α values. Then, for 88 measured Q_α values in SH nuclei, the quantities outside the region of the fit, we obtained an rms deviation of about 250 keV, similar for two treatments of pairing.

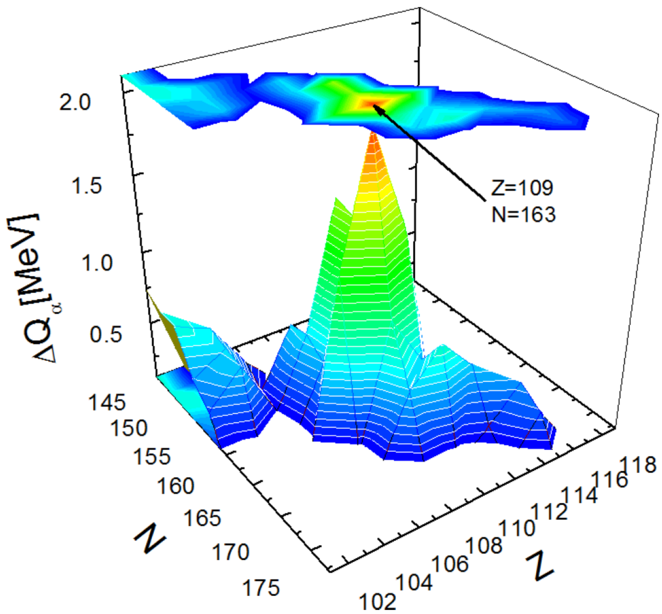

FIG. 1. (Color online) Excitation of the parent g.s. configuration in the daughter nucleus ΔQ_α in isotopes with various Z and N.

III. RESULTS

We also calculated apparent Q_α values, taking the parent g.s. configuration as the final state in the daughter. Such a value is smaller than the true Q_α by the excitation energy of the parent g.s. configuration, ΔQ_α, in the daughter. Global results are collected and shown in Fig. 1. Particularly large—about 2 MeV—excitation of the parent configuration

TABLE I. Predicted high-K ground states in SH nuclei whose excitation in daughter is larger than 0.5 MeV.

Z	N	Ω^p	Ω^n	K^π	ΔQ_α	Z	N	Ω^p	Ω^n	K^π	ΔQ_α
111	169	$9/2^-$	$5/2^+$	7^-	0.74						
111	163	$3/2^-$	$13/2^-$	8^+	1.31	108	163		$13/2^-$	$13/2^-$	1.00
111	161	$3/2^-$	$7/2^+$	5^-	0.52	107	163	$5/2^-$	$13/2^-$	9^+	1.17
110	163		$13/2^-$	$13/2^-$	0.97	107	157	$5/2^-$	$11/2^-$	8^+	0.57
109	169	$11/2^+$	$9/2^+$	10^+	0.51	106	163		$13/2^-$	$13/2^-$	0.96
109	167	$11/2^+$	$5/2^+$	8^+	0.71	105	153	$9/2^+$	$1/2^+$	5^+	0.97
109	166	$11/2^+$		$11/2^+$	0.88	103	157	$7/2^-$	$11/2^-$	9^+	0.52
109	165	$11/2^+$	$3/2^+$	7^+	1.38	103	154	$7/2^-$		$7/2^-$	0.54
109	164	$11/2^+$		$11/2^+$	1.13	103	153	$7/2^-$	$1/2^+$	4^-	1.45
109	163	$11/2^+$	$13/2^-$	12^-	1.99	103	151	$7/2^-$	$9/2^-$	8^+	0.58
109	162	$11/2^+$		$11/2^+$	1.27	103	149	$7/2^-$	$7/2^+$	7^-	0.63
109	161	$11/2^+$	$9/2^+$	10^+	1.32	101	151	$1/2^-$	$9/2^-$	5^+	0.68
109	160	$11/2^+$		$11/2^+$	1.37	101	149	$1/2^-$	$7/2^+$	4^-	0.92
109	159	$11/2^+$	$9/2^+$	10^+	1.56						
109	158	$11/2^+$		$11/2^+$	1.39						
109	157	$11/2^+$	$3/2^+$	7^+	1.41						

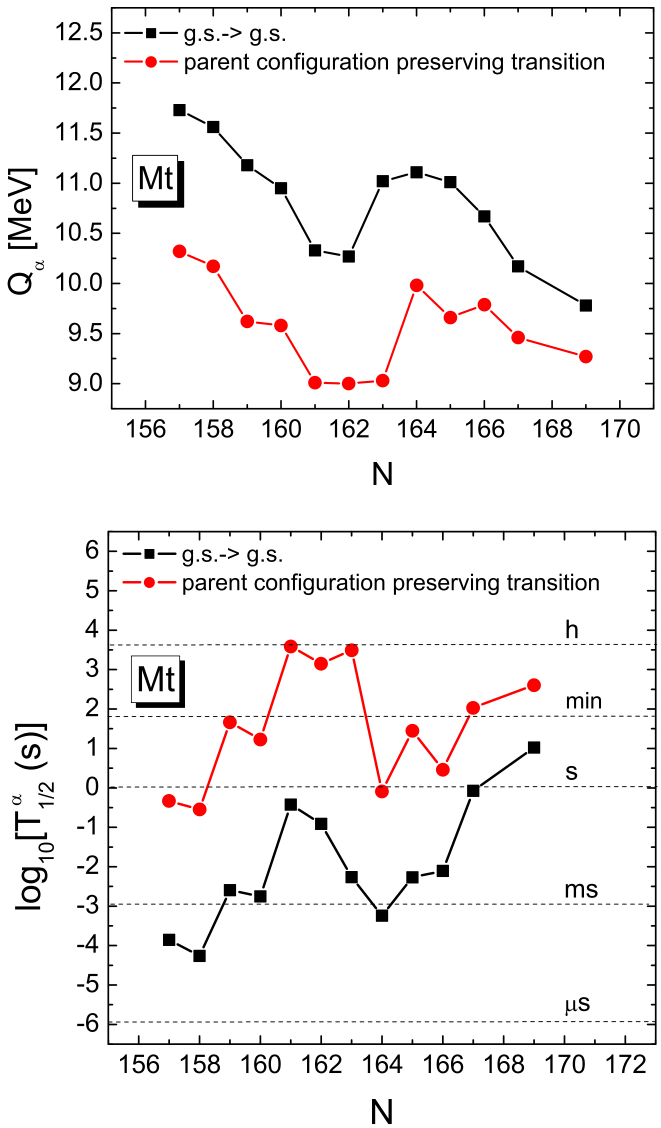

FIG. 2. (Color online) Q_α values calculated with blocking following from the WS model and the increase in α half-life induced by ΔQ_α [29], assuming a complete decay hindrance to different configurations.

occurs in the daughter of ^{272}Mt; an excitation of about 1.5 MeV occurs for ^{256}Lr, thus energies of these configuration-preserving transitions are reduced, especially for particle numbers corresponding to one particle above a closed subshell.

Predicted high-K g.s. configurations in odd and odd-odd SH nuclei whose excitation energy in the daughter is larger than 0.5 MeV are shown in Table I. They result from an interplay between high-j orbital positions and energy minimization. A particular situation occurs at deformed subshells $Z = 102, 108$ and $N = 152, 162$. The levels just above gaps include intruder $\Omega^\pi = 9/2^+$ and $11/2^+$ protons and $11/2^-$ and $13/2^-$ neutrons. It turns out that high-K ground states involving two intruders occur in ^{262}Db and ^{272}Mt. In Table I we shown the g.s. configurations whose excitation in the daughter is larger

TABLE II. Specification of final states in ^{268}Bh for protons (π) and neutrons (ν) with appropriate expectation values $\langle\Sigma^{\pi(\nu)}\rangle$. The corresponding Q_α energies (in MeV) and life-times $\log_{10} T_\alpha$ (in seconds) of ^{272}Mt are shown. The first line concerns ground state to ground state transition.

π state	$\langle\Sigma^\pi\rangle$	ν state	$\langle\Sigma^\nu\rangle$	Q_α	$\log_{10} T_\alpha$
$5/2^-$ [512]	0.93	$9/2^+$ [615]	−0.86	11.02	−2.26
$5/2^-$ [512]	0.93	$7/2^+$ [613]	0.88	10.93	1.97
$5/2^-$ [512]	0.93	$11/2^-$ [725]	0.92	10.64	2.70
$9/2^+$ [624]	0.91	$7/2^+$ [613]	0.88	10.31	3.60
$9/2^+$ [624]	0.91	$11/2^-$ [725]	0.92	10.12	4.14

than 0.5 MeV. It is likely that they have elongated α-decay half-lives.

In Fig. 2, a decrease in energy release, ΔQ_α, and $\log_{10} T_\alpha$ calculated according to [29] for g.s. → g.s. and configuration-preserving transitions are shown for various Meitnerium isotopes. The latter half-life would correspond to an absolute hindrance of configuration-changing decays. For our favorite case, ^{272}Mt, such hindrance reaches six orders of magnitude. This takes us from the life-time of milliseconds to hours.

If one assumes that the configuration hindrance is not absolute but, for example, it amounts to 100 per unpaired nucleon state with the same S_z value (Σ in the Nilsson notation) as in the parent, then one obtains the hindrance factors for various final states in the daughter ^{268}Bh shown in Table II. The orbitals forming the chosen configurations have the expectation value of Σ very close to 1, as both blocked orbitals in the g.s. of ^{272}Mt. Their deformations, obtained by energy minimization, are similar to those for the ground state of ^{268}Bh. The hindrance from the Q_α reduction, HF(ΔQ_α), is included; this means the total hindrance is $10^4 \times$ HF(ΔQ_α). As may be seen, the lowest hindrance corresponds to the configuration nearly degenerate with the ground state. Thus, the result of such an estimate is implied by the assumed configuration hindrance per orbital.

The measured $\log_{10} T_\alpha$ values for Mt isotopes are close to the lower line in Fig. 2, except for $N = 161$ (5 ms [30]) which is below, and $N = 165$ (0.44 s [30]) which is above it. Note that the supposedly isomeric half-life, nearly identical with the lower theoretical point for $N = 161$, was reported [31]. We claim that half-lives corresponding to the upper theoretical curve have not been detected yet, maybe, except for $N = 165$.

Let us stress that the whole argument is based on both the presence of a deformed semimagic shell $Z = 108$ and $N = 162$ and the position of high-Ω intruder orbitals just above that shell. The former is supported by the experimental Q_α values and predictions by many models. The latter is more model -dependent, but the same or nearly the same intruder positions are predicted by the finite range liquid drop model (FRLDM) [27] and the SLy4 Hartree-Fock-Bogoliubov (HFB) model [32].

In order to estimate fission rate for a high-K ground state one can start with the known half-lives of the neighbors and the calculated barriers and half-lives in even-even nuclei [33],

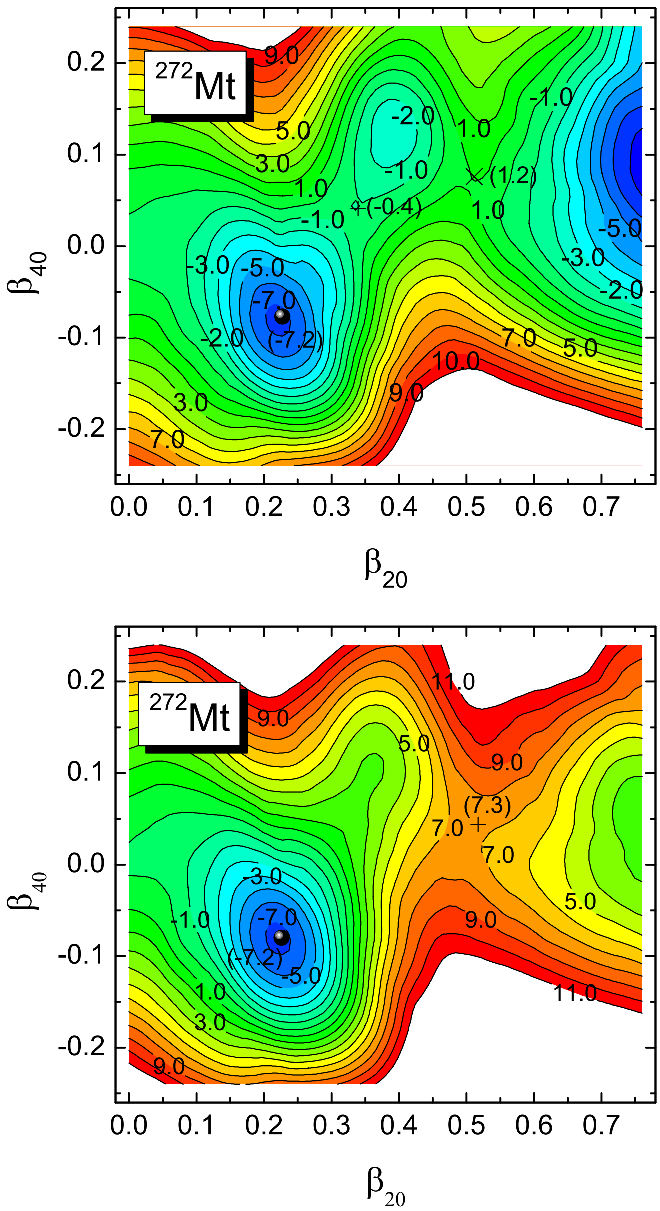

FIG. 3. (Color online) Energy surfaces: $E - E_{\mathrm{mac}}$(sphere) for the ^{272}Mt heavier system in two extreme situations, i.e., adiabatic with minimization over possible configurations (top panel) and nonadiabatic configuration-constrained calculations

and then consider the effect of blocking on the fission barrier and nonadiabatic effects in barrier tunneling.

The experimental half-lives in $N = 163$ isotones are 11 h in ^{266}Lr (s.f.), 1.3 h in ^{267}Rf (s.f.), 30.8 h in ^{268}Db (s.f. + EC), 2 m in ^{269}Sg (α), 3.8 m in ^{270}Bh (α), and 4 s in ^{271}Hs (α). Since the g.s. shell effect in ^{270}Hs is necessarily related to a local barrier maximum [19], its s.f. half-life is in the range of hours [33]. This suggests a spontaneous fission half-life of ^{272}Mt, the odd-odd nucleus, not less than that.

The calculated fission barrier *minimized over configurations* in ^{272}Mt amounts to 6.3 MeV, nearly the same as in ^{270}Hs. The five-dimensional (5D) calculation, including quadrupole nonaxility in addition to four axially- and reflection-symmetric deformations, was done on the hypercube and saddles were obtained by the immersion method. In the nearby even-even isotopes, the nonaxiality in the first barrier was shown to be unimportant [19]. To see the configuration blocking effect, two additional 4D saddle point calculations were performed for axially symmetric deformations in two extreme scenarios: diabatic (with the blocked g.s. configuration) and adiabatic one (minimized over configurations). Also here, saddle points were determined by the immersion method. In Fig. 3 are shown β_{20}, β_{40} energy maps, obtained by minimization over the remaining deformations. One can see a rather dramatic effect of keeping the g.s. configuration: the diabatic saddle point (bottom panel of Fig. 3) lies about 6 MeV higher than the adiabatic one (top panel of Fig. 3). Moreover, there is no second (local) minimum on the diabatic map. We have also checked that the reflection-asymmetry effect on the diabatic/adiabatic saddle is small.

It is known that the blocking procedure often causes an excessive reduction of the pairing gap in systems with odd particle number. One device to avoid an excessive even-odd staggering in nuclear binding was to assume stronger (typically by ∼5%) pairing interaction for odd-particle-number systems; see e.g. [34]. To estimate the effect of a stronger pairing on s.f. barriers we have calculated barriers with pairing strengths increased by 10% and 15%. We obtained still large diabatic fission barriers of 11.8 and 10.3 MeV, respectively.

Obviously, one cannot expect a strict conservation of configuration during the tunneling. It is unavoidable, however, that any configuration change, either related to nonaxiality or to the collective rotation admixture, must induce some increase in the action integral, relative to the neighboring even-even nucleus. Therefore, the fission half-life of the high-K ground state of ^{272}Mt in the range of hours seems to be a safe prediction.

When it comes to β decay, it may be added that the predicted Q_β value of 4.2 MeV in ^{272}Mt means that its β half-life is in the range of minutes [27].

IV. CONCLUSIONS

We summarize as follows:

(i) The macro-micro WS model, which has been shown to give reasonable predictions in the SH region, suggests high-K configurations as the ground states in a number of odd and odd-odd nuclei.

(ii) An α-decay hindrance of such a configuration is expected when the same configuration in the daughter has a sizable excitation. If configuration-changing transitions had been strictly forbidden, the hindrance would have been determined by this excitation ΔQ_α.

(iii) A particular situation occurs above double closed subshells $N = 162$ and $Z = 108$ where two intruder orbitals, neutron $13/2^-$ from $j_{15/2}$ and proton $11/2^+$ from $i_{13/2}$ spherical subshells, are predicted. These orbitals combine to the 12^- g.s. in $Z = 109$, $N = 163$, whose configuration lies ∼2 MeV above the g.s. the daughter. This would imply a six order of magnitude increase in α half-life.

(iv) The double subshell gap at $N = 162$ and $Z = 108$ is consistent with experimental Q_α values and is predicted by many models. The position of neutron $13/2^-$ and proton $11/2^+$ orbitals above this gap is also common to many models; in particular, the predicted g.s. in ^{272}Mt has exactly the same structure in [27]; the same configuration is predicted at $\sim$0.4 MeV excitation within the SLy4 HFB model [32], which would make it also a long-lived one.

(v) The calculated configuration-preserving fission barrier in ^{272}Mt is higher by 6 MeV than the one minimized over configurations. Even if configuration is not completely conserved, a substantial increase in fission half-life is expected.

(vi) There are other orbitals which may produce long-lived configurations, in particular intruder neutron $11/2^-$ and proton $9/2^+$ above $N = 152$, $Z = 102$. Although more model dependent, there is a possibility that one such high-K ground or low-excited state may be the longest-lived superheavy nucleus.

As already mentioned, one cannot exclude that such long-lived superheavy configurations were already produced before, but setup and electronics dedicated to the milliseconds measurements could not detect decays of objects living much longer. This intriguing possibility should be checked first.

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