

# Multi-quasiparticle excitation: Extending shape coexistence in $A \sim 190$ neutron-deficient nuclei

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## Abstract

Multi-quasiparticle high- $K$  states in neutron-deficient mercury, lead, and polonium isotopes have been investigated systematically by means of configuration-constrained potential-energy-surface calculations. An abundance of high- $K$  states is predicted with both prolate and oblate shapes, which extends the shape coexistence of the mass region. Well-deformed shapes provide good conditions for the formation of isomers, as exemplified in  $^{188}\text{Pb}$ . Of particular interest is the prediction of low-lying  $10^-$  states in polonium isotopes, which indicate long-lived isomers.

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## I. INTRODUCTION

The shape-coexistence phenomenon in the  $A \sim 80$  and 190 mass regions has been a subject of considerable interest over a number of years [1–3]. Recent experimental progress in the identification of low-lying shape-coexisting  $0^+$  states in  $^{186}\text{Pb}$  has led to renewed interest in this topic [4]. Indeed, the shape coexistence in lead nuclei around  $N = 104$  may represent one of the most dramatic manifestations of this phenomenon. Due to the presence of the  $Z = 82$  shell closure, the ground states (g.s.) of neutron-deficient lead isotopes are dominated by sphericity, with two different shapes (oblate and prolate) coexisting at low excitation energies ( $\lesssim 3$  MeV). For even-even nuclei, one of the most important experimental fingerprints of shape coexistence is the observation of different low-lying  $0^+$  states with respective rotational bands. At least one low-lying  $0^+$  state with excitation energy below 1.0 MeV has, to date, been observed in all even-even lead isotopes with neutron number ranging from 100 to 112. Rotational bands based on both prolate [5–7] and oblate [8, 9] shapes have been observed in  $^{186,188}\text{Pb}$ .

From a shell-model point of view, the appearance of low-lying excited  $0^+$  states in lead isotopes stems from proton 2p-2h and 4p-4h (or 6p-6h) excitations across the  $Z = 82$  shell closure. Potential-energy-surface (PES) calculations, however, show rather soft deformations for neutron-deficient lead and polonium isotopes, indicating considerable mixing between bands with different shapes (see e.g., [10, 11]). This has been confirmed experimentally by the observation of  $E0$  components in  $J \rightarrow J$  transitions at low spins between bands that arise from different shapes in  $^{188}\text{Pb}$  [12], which is known to be a signature of shape mixing [13]. The mixing between different shapes is itself an interesting issue, although this may lead to considerable difficulty in isolating different shapes. One should notice that it is the shape mixing that complicates significantly the shape interpretations of the low-lying band structures in light polonium isotopes [3, 14]. In practice, a two- or three-level-mixing analysis [15, 16] or even a more sophisticated model [17, 18] is needed to account for the shape mixing.

The shallow (soft) deformed sub-minima in the PES can be stabilized by collective rotation that can cause Coriolis mixing of high- $j$  orbits which have strong deformation-driving effects. To increase the stability of soft deformation, another mechanism, that is discussed in the present work, is multi-quasiparticle excitation which can cause shape polarization due

to unpaired nucleons. It is shown that the occupation of high- $\Omega$  orbits by unpaired nucleons can polarize the nuclei to be strongly deformed [19]. Well-deformed axial shapes, combined with low excitation energies, give good conditions for the formation of high- $K$  isomers [20]. Due to the possibility of increased stability, isomeric states in the unstable neutron-deficient nuclei would be advantageous for experimental measurements, with their decays providing useful structure information [12]. Indeed, significant progress has been made in the measurement of isomers in the most neutron-deficient lead isotopes [3]. In  $^{188}\text{Pb}$ , for example, three spin-isomers with different shapes have been identified and characterized by measuring rotational bands built upon them [12, 21].

Another interesting feature in this mass region is the occurrence of oblate-deformed high- $K$  isomers arising from the filling of strongly oblate-driving high- $\Omega$  orbits. Compared to prolate shape, it is rare for nuclei to have oblate deformation. The importance of oblate shapes is not only due to their rare occurrence, but also because the small number of oblate shapes may have a direct link to the detailed form of the mean-field potential [22, 23]. The observation of a region of nuclei with stable oblate shapes would thus form an interesting testing ground for various mean-field models. Moreover, insight into the shell structure of nucleon orbits at oblate shape can be obtained from the excitation energies and configurations of isomers.

In this work we investigate the shape-coexistence phenomenon of two-quasiparticle isomeric states in the  $A \sim 190$  mass region at both prolate and oblate deformations by means of configuration-constrained PES calculations. At oblate shapes, we give predictions of high- $K$  states in neutron-deficient lead and polonium isotopes. At prolate deformations, our main attention has been paid to systematic prediction of isomers in the  $N = 102$  and  $104$  isotones. For this purpose, we extend our calculations to the lighter  $N = 102$  and  $104$  isotones where more experimental information is available. Another motivation of the present work is to study the shape polarization effect from multi-quasiparticle excitations.

## II. THE MODEL

We have used the macroscopic-microscopic model with the standard liquid-drop energy [24] and microscopic shell and pairing corrections. Single-particle levels which are needed in the calculation of the microscopic energy are given by the nonaxial deformed

Woods-Saxon (WS) potential with the set of universal parameters [25]. In order to avoid the possible collapse of pairings in multi-quasiparticle states, the approximate particle-number conservation by means of the Lipkin-Nogami (LN) pairing [26] has been employed with monopole pairing considered. The energy calculation of the macroscopic-microscopic model is standard as given, e.g., in Ref. [27]. For a multi-quasiparticle state, however, the microscopic energy contains the contribution from the unpaired particles which occupy the single-particle orbits specified by the given configuration, see our previous work [28] for the detailed formula. Blocking effects from the unpaired particles are taken into account by removing the configuration orbits in the LN pairing calculation.

In the macroscopic-microscopic model, the deformation of a state is obtained by minimizing the corresponding PES. The configuration-constrained PES calculation [28] for a multi-quasiparticle state requires the adiabatic blockings of the configuration orbits in the considered deformation space  $(\beta_2, \gamma, \beta_4)$ , i.e., the specific single-particle orbits are kept singly occupied while changing the deformation in the PES calculation. This has been achieved by calculating and identifying the average Nilsson quantum numbers of every orbit involved in the configuration [28]. The energy of a multi-quasiparticle state can be decomposed into the deformation energy and the configuration energy which corresponds to the quasiparticle excitations that undergo the pair breakings and excitations of the particles involved in the configuration. Due to the polarization of the quasiparticle excitations, the deformation of a multi-quasiparticle state can be different from the one of the ground state. The shape polarization can be significant in a deformation-soft nucleus and result in a remarkably different deformation energy from that of the ground state. It has been shown that the self-consistent energy-deformation calculation by means of the configuration-constrained PES is very powerful to give the right deformation and energy of a multi-quasiparticle state [19, 28]. In the present model, the excitation energy which can be compared with the experimental energy is obtained by the energy difference between the minima of the multi-quasiparticle and ground-state PES's. We will discuss more about the calculations of excitation energies which are important for predictions or comparisons with experimental data.

The pairing strength,  $G$ , is an important fact that affects the energy calculation [28]. As done in previous works [19, 28], the pairing strength ( $G$ ) is determined firstly by the average gap method [29] and then adjusted to reproduce the experimental odd-even mass difference using a five-point formula in both experiment and theory. For nuclei in the valley of magic

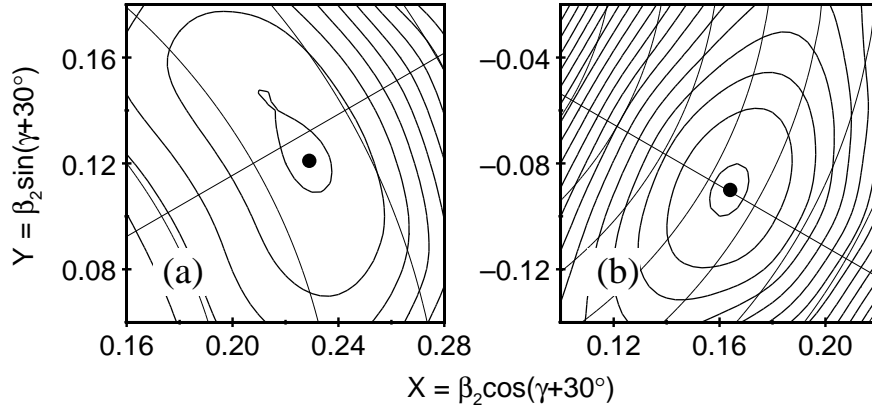


FIG. 1: Configuration-constrained PES's for the *prolate*  $K^\pi = 6^-$  ( $\nu\{7/2[633], 5/2[512]\}$ ) state (a) and the *oblate*  $K^\pi = 11^-$  ( $\pi\{13/2[606], 9/2[505]\}$ ) state (b) in  $^{186}\text{Pb}$ . The calculated deformations and excitation energies can be found in Tables I and III. The energy difference between neighbouring contours is 100 keV. The intrinsic PES's are reflection-symmetric about  $\gamma = 0^\circ$ , i.e., the shape with  $\gamma = -60^\circ$  is the same as the one with  $\gamma = 60^\circ$  for non-collective excitations.

numbers, however, it has been pointed out that there are irregularities in the mass difference and thus the shell-closed nuclei are excluded in the determination of pairing strength [29]. Therefore, we take the standard  $G$  [29] for lead and polonium isotopes.

### III. CALCULATIONS AND DISCUSSIONS

$K^\pi = 11^-$ ,  $\pi\{9/2^-[505], 13/2^+[606]\}$ , isomers have been observed systematically in even-even  $^{188-196}\text{Pb}$  and  $^{194-210}\text{Po}$  [3], with the configuration confirmed by g-factor measurements in  $^{196}\text{Pb}$  [30] and  $^{198,200}\text{Po}$  [31].  $K^\pi = 8^+$  isomers have also been found experimentally in  $^{188-196}\text{Pb}$  and  $^{198-210}\text{Po}$  [3]. The configuration of the  $8^+$  isomers has been assigned to be  $\pi\{9/2^-[505], 7/2^-[514]\}$  confirmed also by g-factor measurements in  $^{198,200}\text{Po}$  [31]. The proton Nilsson diagram shows that many oblate-driving high- $\Omega$  orbits appear around the Fermi surface of  $Z \approx 82$  at the oblate side of  $\beta_2 \approx 0.2$ , which has been seen in the neighbouring odd- $Z$  nuclei as isomeric states. It may be expected that high- $K$  states with even lower energies and larger deformations could exist in polonium isotopes since the proton Fermi level for  $Z = 84$  is located amongst these high- $\Omega$  orbits.

We have performed systematic calculations for lead and polonium isotopes with  $N = 104 - 116$ . Table I lists the detailed results for the oblate isomers in lead isotopes, includ-

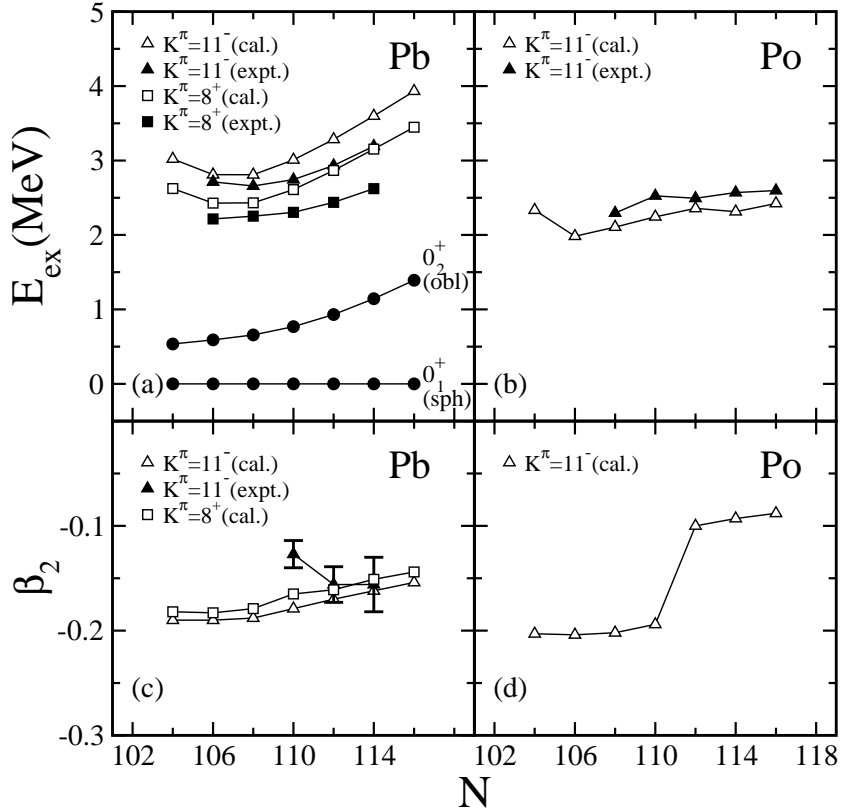


FIG. 2: Excitation energies (panels (a) and (b)) and the corresponding  $\beta_2$  deformations (panels (c) and (d)) for  $\pi\{13/2^+[606], 9/2^-[505]\}$  ( $K^\pi = 11^-$ ) and  $\pi\{7/2^-[514], 9/2^-[505]\}$  ( $K^\pi = 8^+$ ) oblate states in lead and polonium isotopes. The experimental data are from Refs. [3, 32, 33]. In panel (a), the black dots give the experimental energies of the  $0_1^+$  (spherical) and  $0_2^+$  (oblate) states.

ing available experimental energies. As examples, Fig. 1 displays configuration-constrained PES's for the predicted prolate  $6^-$  and oblate  $11^-$  states (the prolate states will be discussed later). For systematic comparisons, we plot energies and deformations which can be obtained experimentally in Fig. 2 for the oblate states. It can be seen that the overall agreement between calculations and data for the observed  $11^-$  and  $8^+$  isomers in lead isotopes is reasonably good. The calculations reproduce the experimental behaviour of energies changing with neutron number, but overestimate the energies in heavier lead isotopes. The discrepancy between measurements and calculations grows from about 100 keV in  $^{188}\text{Pb}$  to 500 keV in  $^{196}\text{Pb}$ . The oblate  $|\beta_2|$  values for the  $11^-$  and  $8^+$  isomers in lead isotopes decrease smoothly from 0.19 in  $^{186}\text{Pb}$  to 0.15 in  $^{198}\text{Pb}$ . For comparison, three available experimental  $\beta_2$  values extracted from the measured spectroscopic quadrupole moments in

$^{192-196}\text{Pb}$  [32, 33] are given. We see that the calculations reproduce well the experimental deformations in  $^{194,196}\text{Pb}$ , but give a smaller deformation in  $^{192}\text{Pb}$ . The energies and deformations obtained in the present work are consistent with previous Nilsson-Strutinsky [10] and Skyrme-HFB [33, 34] calculations which were limited to axially symmetric shapes.

TABLE I: Calculated excitation energies and deformations of the oblate two-quasiparticle isomeric states in lead isotopes. The experimental energies and quadrupole moments can be found in Refs. [3, 32, 33] and references therein. Note that a negative  $\beta_2$  value corresponds to a  $\gamma = 60^\circ$  oblate shape.

Nuclei	$K^\pi$	Configurations	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$Q_{20}^{expt.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
$^{186}\text{Pb}$	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.19	0.01	-5.34		3021	
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.21	0.01	-6.54		3482	
	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.18	0.01	-5.71		2623	
$^{188}\text{Pb}$	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.18	0.00	-5.80		2638	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.19	0.01	-5.42		2810	2713
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.22	0.01	-6.77		3268	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.18	-0.01	-5.75		3898	
	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.18	0.01	-5.72		2428	2216
$^{190}\text{Pb}$	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.17	0.00	-5.71		2764	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.19	0.00	-5.46		2809	2658
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.22	0.01	-6.70		3300	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.18	-0.01	-5.72		3840	
	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.18	0.01	-5.76		2431	2252
$^{192}\text{Pb}$	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.18	0.00	-5.37	-3.5(4)	3009	2743.5

Continued. . .

TABLE I – continued

Nuclei	$K^\pi$	Configurations	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$Q_{20}^{cal.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
$^{194}\text{Pb}$	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.21	0.00	-6.49		3606	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.17	-0.02	-5.58		3928	
	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.17	0.00	-5.22		2609	2304
	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.17	-0.01	-5.15	-4.3(5)	3284	2933
$^{196}\text{Pb}$	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.16	0.00	-4.89		2867	2437.4
	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.16	-0.01	-4.74	-4.1(8)	3598	3192.2
$^{198}\text{Pb}$	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.15	-0.01	-4.70		3153	2621.9
	$0^+$	g.s.	0.01	0.00	0.00		0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.15	-0.02	-4.36		3931	
	$8^+$	$\pi\{9/2^-[505], 7/2^-[514]\}$	-0.14	-0.01	-3.88		3447	

Compared with the situation in the lead isotopes, the shape-coexistence phenomenon is less established in the polonium isotopes. For the lead isotopes investigated, the ground states are always spherical and the  $0_2^+$  states have oblate shapes, as shown in Fig. 2. This is consistent with results given by the Skyrme-HFB calculations [34]. For the polonium isotopes, the PES's are more complicated. Fig. 3 displays potential energy curves as the function of  $\beta_2$  deformation. At each  $\beta_2$  point, the energy has been minimized with respect to the  $\beta_4$  parameter. We see that the seniority-zero  $0^+$  energy curves are very soft against deformations, which is consistent with the experimental observation of the vibrational property of low-lying states in  $^{194,196}\text{Po}$  [35]. In Ref. [3], it was commented that the low-lying states would have shape mixing with 2p and 4p-2h configurations. Our calculations show oblate minima at  $\beta_2 \approx -0.2$  in  $^{188-196}\text{Po}$  and prolate minima at  $\beta_2 \approx 0.25$  in  $^{188,190}\text{Po}$ . Weak and soft deformations with  $|\beta_2| < 0.1$  exist in the polonium isotopes, which would indicate nearly spherical shapes. The calculated energy curves are in general similar to those obtained by Skyrme-HFB model [34], giving similar conclusions about shape coexistences in the isotopes. These calculations are also consistent with the previous PES calculations [16].



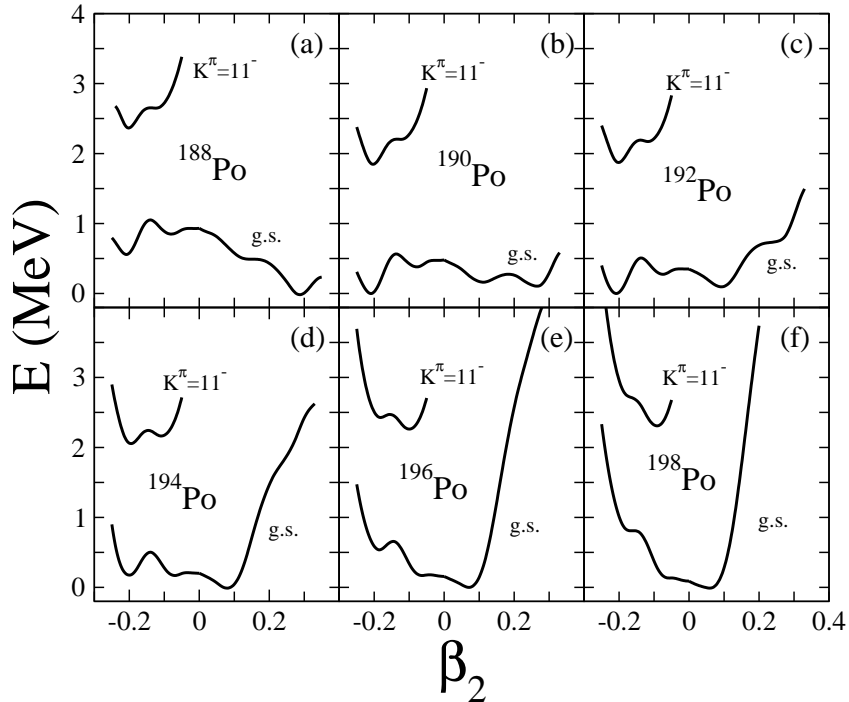


FIG. 3: Potential energy curves against  $\beta_2$  deformation for seniority-zero  $K^\pi = 0^+$  (i.e., no quasi-particle excitation) and two-quasiproton  $\pi\{13/2^+[606], 9/2^-[505]\}$   $K^\pi = 11^-$  states in neutron-deficient even-even polonium isotopes. The lowest minimum in the seniority-zero curve (marked by g.s.) gives the ground state.

Experimentally, the lowest  $2^+$  and  $4^+$  states in heavier polonium isotopes with  $N \geq 116$  have approximately constant excitation energies [3]. These nuclei can be considered as nearly-spherical anharmonic vibrators [3]. For even-even polonium isotopes lighter than  $^{198}\text{Po}$ , the energies of the yrast band members undergo a progressive decrease with decreasing neutron number (e.g., see Fig. 24 of Ref. [3]). This has been taken as evidence that the systems start to evolve towards more collectivity through mixing [36], which is consistent with our calculations in which oblate minima arise in the isotopes lighter than  $^{198}\text{Po}$ . Recent experiments have confirmed the mixing scenario in  $^{194}\text{Po}$  [14]. For  $^{190}\text{Po}$ , low-lying band structure with prolate shape has been observed [37], which is also consistent with our calculation.

TABLE II: Similar to Table I, but for polonium isotopes.

Nuclei	$K^\pi$	Configurations	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
$^{188}\text{Po}$	$0^+$	g.s.	0.29	0.01	10.86	0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.20	0.01	-6.01	2422	
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.21	0.02	-6.92	1697	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.20	0.01	-6.01	3307	
	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.21	0.01	-6.54	2843	
$^{190}\text{Po}$	$0^+$	g.s.	-0.21	0.01	6.78	0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.21	-0.01	-6.87	1611	
	$6^-$	$\nu\{7/2^+[633], 5/2^-[503]\}$	-0.20	0.00	-6.46	2269	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.20	0.01	-6.49	1960	
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.21	0.02	-6.94	1212	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.21	0.00	-6.10	2830	
	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.21	0.01	-6.56	2352	
$^{192}\text{Po}$	$0^+$	g.s.	-0.20	0.00	-6.70	0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.20	-0.01	-6.55	1839	
	$6^-$	$\nu\{7/2^+[633], 5/2^-[503]\}$	-0.21	0.00	-6.71	1710	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.20	0.01	-6.49	1923	
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.21	0.01	-7.01	1168	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.20	0.00	-6.00	2771	
	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.21	0.01	-6.49	2300	
$^{194}\text{Po}$	$0^+$	g.s.	0.07	0.01	2.90	0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.08	-0.01	-2.93	2087	
	$6^+$	$\nu\{7/2^+[633], 5/2^+[642]\}$	-0.20	0.00	-6.43	1668	
	$6^-$	$\nu\{7/2^+[633], 5/2^-[503]\}$	-0.20	0.00	-6.43	1721	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.19	0.00	-5.93	2096	2525.2
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.21	0.01	-6.69	1381	

Continued...

TABLE II – continued

Nuclei	$K^\pi$	Configurations	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
$^{196}\text{Po}$	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.19	-0.01	-6.42	2910	
	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.20	0.01	-6.14	2489	
	$0^+$	g.s.	0.06	0.00	2.51	0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.08	-0.01	-2.78	2190	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.10	0.02	-3.66	2287	2493
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.19	0.01	-6.03	1825	
	$10^-$	$\pi\{11/2^+[615], 9/2^-[505]\}$	-0.18	-0.02	-5.94	3206	
$^{198}\text{Po}$	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.19	0.00	-6.25	2874	
	$0^+$	g.s.	0.06	0.00	2.21	0	0
	$8^+$	$\nu\{9/2^+[624], 7/2^+[633]\}$	-0.07	-0.01	-2.94	2289	
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.10	0.01	-3.40	2302	2565.9
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.18	0.00	-5.89	2199	
$^{200}\text{Po}$	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.18	0.01	-6.12	3169	
	$0^+$	g.s.	0.05	0.00	1.92	0	0
	$11^-$	$\pi\{13/2^+[606], 9/2^-[505]\}$	-0.09	0.01	-3.30	2423	2596
	$10^-$	$\pi\{13/2^+[606], 7/2^-[514]\}$	-0.17	0.00	-5.84	2629	
	$9^-$	$\pi\{11/2^+[615], 7/2^-[514]\}$	-0.17	-0.01	-5.70	3534	

Now we investigate multi-quasiparticle states in the polonium isotopes. We have made detailed theoretical search for possible low-lying two-quasiparticle high- $K$  states, given in Table II with calculated excitation energies and deformations. The two-quasiproton  $\pi\{13/2^+[606], 9/2^-[505]\}$   $K^\pi = 11^-$  states are of particular interest, which have been observed experimentally to be isomers in  $^{194-200}\text{Po}$  and investigated extensively in both experiments [3] and theories [10, 34]. The experimental excitation energies of the  $11^-$  isomers are about 2.5 MeV. A recent experiment observed a 580(100) ns isomer deexciting via a 154 keV transition to the  $10^+$  member of the collective band in  $^{192}\text{Po}$  [38]. The  $E1$  multipolarity of the 154 keV transition is indicative of an  $11^-$  isomer at an excitation energy of 2295 keV. The calculated configuration-constrained PES's are displayed in Fig. 3. We see that the  $11^-$

isomeric states have soft oblate shapes. In  $^{194}\text{Po}$  case, it seems that there are two minima at  $\beta_2 \approx -0.2$  and  $\beta_2 \approx -0.1$ , respectively, with a low barrier between them. From  $^{194}\text{Po}$  to  $^{196}\text{Po}$ , the lowest minimum moves from  $\beta_2 \approx -0.2$  to  $\beta_2 \approx -0.1$ , respectively, which has also been shown in Fig. 2. However, this would not imply a real abrupt change of the deformation. It would be more reasonable to conclude that the  $11^-$  states in  $^{194,196}\text{Po}$  have soft oblate deformations with  $\beta_2$  between  $-0.2$  and  $-0.1$ .

It has been explained that the excitation energy is obtained in the present model by the energy difference between the minima of the multi-quasiparticle and ground-state PES's. For deformation-soft states, however, the configuration mixing (or called deformation mixing) would be remarkable [34]. The authors of Ref. [34] have performed configuration-mixing calculations within the generator coordinate method (GCM) for the  $0^+$  states of the shape-soft polonium isotopes, giving that the mixing can make eigen energies deviate from the PES minima. However, we notice that the energy difference between the  $0_2^+$  and  $0_1^+$  eigen states obtained in the GCM calculations is in general similar to the energy difference between the second and first minima given by the PES [34]. *← Phil: is it dangerous or necessary to give this comment?* In the present model, we may expect that deformation-mixing effects on energies are canceled at least partly due to the similar softnesses of the seniority-zero  $0^+$  and two-quasiparticle  $11^-$  PES's near the minima. Therefore, the excitation energy obtained by the PES minima should be an acceptable approximation for a multi-quasiparticle state. This has been well testified in our calculations including the previous works [19, 28], compared with experimental data. The lead isotopes have well-defined spherical ground states and oblate multi-quasiparticle states. In Ref. [34] the PES minima have been taken in the determinations of energies and deformations for the lead isotopes, which has also been justified by configuration-mixing calculations [39–42], indicating that deformation-mixing effect is less significant in the isotopes. Therefore, the calculations of excitation energies by PES minima should be more accurate for the multi-quasiparticle states of the lead isotopes.

Fig. 2 shows comparisons with experimental energies for the  $K^\pi = 11^-$  isomeric states. We see that experimental energies are reproduced reasonably. In the lead isotopes, the  $11^-$  isomers (and also the  $8^+$  isomers) have a trend of increasing energy with neutron number, in a similar way to the oblate  $0_2^+$  states, see Fig. 2. This is easily understood because the isomers are built on the oblate minima. Experiments have confirmed that the oblate  $0_2^+$  states are always higher than the spherical  $0_1^+$  states and the energies increase monotonically with

increasing neutron number (shown in Fig. 2). In the polonium isotopes, the deformation-soft  $11^-$  states are also constructed on oblate minima, while the situation for the  $0^+$  minima are complicated with the possible coexistence of oblate, prolate and nearly spherical shapes as discussed above. The systematic underestimation of  $\approx 200 - 400$  keV in the polonium isotopes may indicate the effect from the deformation mixing. However, as another possibility which has been observed in the previous works [19, 28], systematic discrepancies between calculated and experimental energies would be related to pairing strengths taken in the present model. A slight increase of the pairing strength can significantly increase the excitation energies of multi-quasiparticle states [19, 28]. The systematic overestimation for the energies of the  $11^-$  and  $8^-$  isomers in the lead isotopes can be explained by a slight decrease of the proton pairing strength.

In addition to the  $11^-$  and  $8^+$  isomers observed systematically, we see in Tables I and II that many other two-quasiparticle high- $K$  states are predicted to exist in the neutron-deficient lead and polonium isotopes with excitation energies lower than 3.5 MeV. Of particular interest is that in the polonium isotopes the two-proton  $10^-$  states with the configuration of  $\pi\{13/2^+[606], 7/2^-[514]\}$  are predicted to have lower energies than other two-quasiparticle states including the observed  $11^-$  isomers. The low excitation energies indicate the possibility of long-lived  $10^-$  states which it would be interesting to observe in future experiments. The high- $K$  states provide good laboratories for the study of oblate deformations and the shape-coexistence phenomenon in the neutron-deficient lead and polonium isotopes.

For a multi-quasiparticle state, the quadrupole moment and  $g$  factor are other important observables which provide direct information on the deformation and configuration. In the present model, the intrinsic quadrupole moment is calculated by  $Q_{20} = \sum q_{k_j} + \sum_{k \neq k_j} 2V_k^2 q_k$ , where  $q_k$  is the single-particle quadrupole moment of the  $k$ -th orbit given in the WS model. The first term gives the contribution from the unpaired particles which stay on the  $k_j$ -th orbit, and the second term is from all the paired particles which occupy the WS orbits with probabilities  $V_k^2$  in the LN pairing model. Blocking effects are taken into account by restricting  $k \neq k_j$  in the sum. The quadrupole moment thus calculated is configuration-dependent. In Tables I, II and III, we predict quadrupole moments for multi-quasiparticle and ground states. The present model has not been available for the calculation of the  $g$  factor, but we will make the improvement.

Experimental information concerning prolate high- $K$  isomers in mercury and lead iso-

topes is relatively scarce. The only known cases are the two-quasineutron  $K^\pi = 8^-$  ( $\nu\{7/2^-[514], 9/2^+[624]\}$ ) states observed in  $^{186}\text{Hg}$  [43] and  $^{188}\text{Pb}$  [12] with  $N = 106$ . In the  $N = 104$  isotones, the dominance of the  $8^-$  intrinsic state is taken over by the favoured  $K^\pi = 6^+$  ( $\nu\{7/2^-[514], 5/2^-[512]\}$ ) and  $7^-$  ( $\nu\{7/2^+[633], 7/2^-[514]\}$ ) states. The  $6^+$  isomers have been observed from  $^{172}\text{Er}$  to  $^{180}\text{Os}$  with half-lives ranging from several  $\mu\text{s}$  to a few ns [44, 45]. The  $7^-$  isomers have been seen in  $^{178}\text{W}$  [46],  $^{180}\text{Os}$  [47], and  $^{182}\text{Pt}$  [48]. For  $N = 102$  isotones, a  $K^\pi = 6^-$  state with the configuration of  $\nu\{7/2^+[633], 5/2^-[512]\}$  was observed in  $^{172}\text{Yb}$  [49],  $^{174}\text{Hf}$  [50], and probably  $^{170}\text{Er}$  [51]. These three configurations have not been observed in the heavier isotones of  $N = 104$  and  $102$ , although similar band structure that might be associated with a  $K$  isomer has been observed in  $^{184}\text{Hg}$  [52]. We note that the  $K^\pi = 6^-$   $\nu\{7/2^+[633], 5/2^-[512]\}$  configuration has an unfavored residual spin-spin interaction ( $\approx +300$  keV) while the residual interaction is favored for the  $6^+$ ,  $7^-$ , and  $8^-$  configurations ( $\approx -100$  keV) [53]. This would be a reason why the  $6^-$  state is more difficult to observe compared with the neighbouring  $6^+$ ,  $7^-$ , and  $8^-$  states. The residual interactions are not included in the present calculations. In Ref. [19], the structures of the two-neutron  $8^-$  ( $\nu\{9/2^+[624], 7/2^-[514]\}$ ) isomers which have been observed systematically in the  $N = 106$  isotones in this mass region were calculated, showing remarkable shape changes with proton number approaching the  $Z = 82$ . The quasiparticle excitations provide useful information about the shell structure of nucleon orbits. The calculations of high- $K$  states, particularly the predictions of energies, can provide important guidance for future experimental investigations.

TABLE III: Calculated excitation energies and deformations of the two-quasineutron  $7^-$ ,  $6^-$ , and  $6^+$  states in  $N = 102$  and  $N = 104$  isotones, with the configurations of  $\nu\{7/2^+[633], 7/2^-[514]\}$ ,  $\nu\{7/2^+[633], 5/2^-[512]\}$ , and  $\nu\{7/2^-[514], 5/2^-[512]\}$ , respectively.  $\gamma \approx 0^\circ$  for all the states except the  $^{184}\text{Pb}$   $6^+$  state which has  $\gamma \approx 15^\circ$ . The experimental energies can be found in Refs. [46, 48, 54] and references therein.

Nuclei	$K^\pi$	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
$^{176}_{74}\text{W}_{102}$	$7^-$	0.30	-0.02	9.29	1786	
	$6^-$	0.27	-0.01	8.15	1531	

Continued...

TABLE III – continued

Nuclei	$K^\pi$	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
$^{178}_{74}\text{W}_{104}$	$6^+$	0.25	-0.02	7.50	1795	
	$7^-$	0.25	-0.03	7.49	1696	1738
	$6^-$	0.25	-0.02	7.52	1860	
$^{178}_{76}\text{Os}_{102}$	$6^+$	0.26	-0.03	7.78	1594	1665
	$7^-$	0.22	-0.02	6.43	1870	
	$6^-$	0.24	-0.01	7.33	1766	
$^{180}_{76}\text{Os}_{104}$	$6^+$	0.22	-0.02	6.43	1873	
	$7^-$	0.22	-0.03	6.56	1816	1930
	$6^-$	0.22	-0.02	6.46	1954	
$^{180}_{78}\text{Pt}_{102}$	$6^+$	0.23	-0.03	6.90	1832	1878
	$7^-$	0.23	-0.01	7.16	1981	
	$6^-$	0.25	0.00	8.07	1827	
$^{182}_{78}\text{Pt}_{104}$	$6^+$	0.23	-0.01	7.16	1981	
	$7^-$	0.23	-0.02	7.09	1989	1955
	$6^-$	0.23	-0.01	7.25	2053	
$^{182}_{80}\text{Hg}_{102}$	$6^+$	0.25	-0.03	8.00	2020	
	$7^-$	0.25	0.00	8.39	2075	
	$6^-$	0.26	0.00	8.90	1853	
$^{184}_{80}\text{Hg}_{104}$	$6^+$	0.24	0.00	7.93	2094	
	$7^-$	0.24	-0.01	7.99	2285	
	$6^-$	0.25	-0.01	8.39	2452	
$^{184}_{82}\text{Pb}_{102}$	$6^+$	0.26	-0.01	8.83	2094	
	$7^-$	0.27	0.01	10.15	2296	
	$6^-$	0.27	0.01	10.15	1978	
$^{186}_{82}\text{Pb}_{104}$	$6^+$	0.26	0.01	9.72	2300	
	$7^-$	0.26	-0.01	9.50	2659	

Continued...

TABLE III – continued

Nuclei	$K^\pi$	$\beta_2$	$\beta_4$	$Q_{20}^{cal.}$ (eb)	$E_{ex}^{cal.}$ (keV)	$E_{ex}^{expt.}$ (keV)
	$6^-$	0.26	-0.01	9.50	2846	
	$6^+$	0.27	-0.01	10.04	2310	

We therefore made a thorough search for a variety of possible multi-quasiparticle states along the  $N = 104$  and  $102$  isotonic chains with  $Z = 74 - 82$ . Similar PES calculations for the  $6^+$  states have been reported in some  $N = 104$  isotones [45]. The detailed calculations of energies and deformations are listed in Table III. For clear comparisons of energies and deformations, see also Fig. 4. Good agreements between experiments and calculations are obtained for the known  $6^+$  and  $7^-$  states in the  $N = 104$  isotones. Note that the observed  $7^-$  1.93 MeV state in  $^{180}\text{Os}$  is expected to mix with the  $7^-$  1.86 MeV member of a side band [47]. The unperturbed levels should then lie closer. As an interesting example, the nucleus  $^{186}\text{Pb}$  is calculated to have a spherical ground state, and several prolate and oblate high- $K$  states (see Fig. 1).

While almost all the ground states of the studied lead and polonium isotopes have relatively small deformations except for the polonium isotopes lighter than  $^{194}\text{Po}$ , nearly all the calculated high- $K$  states have well-deformed axial shapes (see Tables I and II), indicating significant shape polarizations from the pair-broken nucleons. Further, we found that the orbital blockings can stabilize the minimum of the configuration-constrained PES for these nuclei. The effect on the stability of states has also been seen in the superheavy nuclei where unpaired nucleons lead to higher and wider fission barriers for high- $K$  states as compared to the respective ground states [55]. Compared with the ground states which have soft deformations, these relatively rigid high- $K$  states are less susceptible to shape mixing, thus providing good opportunities for the study of shape coexistence in this mass region. Due to the fact that the neutron-deficient polonium isotopes are close to the proton dripline and due to the predominant fission channel, spectroscopic studies of these nuclei become increasingly difficult. The present calculations suggest that it may be possible to investigate these nuclei via the measurements of the high- $K$  isomers. Experimentally, the shape-polarization effect that leads to larger deformation and more rigid shapes has been seen in odd-mass polonium isotopes in  $\alpha$ -decay studies. In  $^{191}\text{Po}$ , for example, two  $\alpha$ -decaying isomers were observed



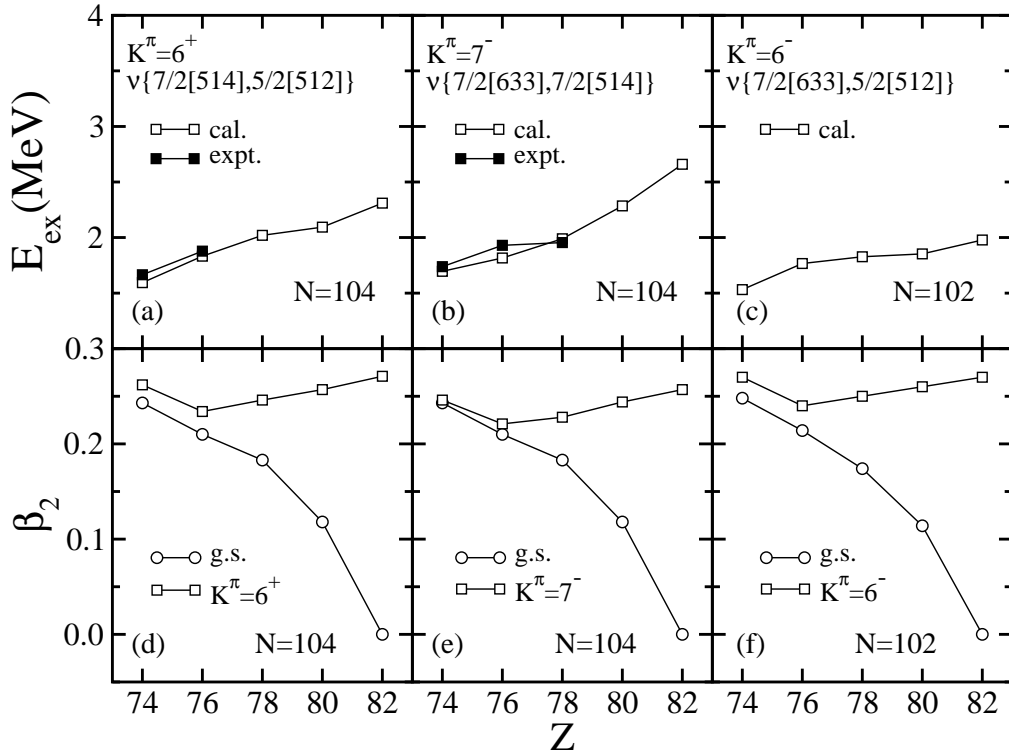


FIG. 4: Similar to Fig. 2, but for prolate high- $K$  states in  $N = 104$  and  $102$  isotones.

to have remarkably different half-lives, which has been interpreted to be due to the large shape polarization from the odd nucleon. The authors of Ref. [56] noticed also that the longer-lived isomeric state is purer as compared to the even-even neighbours. The observed low-spin band structures based on high- $K$  orbits in odd-mass polonium isotopes have also shown more pronounced collectivity than in the neighbouring even-even isotopes [57].

#### IV. SUMMARY

Configuration-constrained PES calculations have been performed to investigate the shape-coexistence phenomenon associated with high- $K$  states in neutron-deficient mercury, lead, and polonium isotopes. A large number of oblate-shape high- $K$  states are predicted to occur at low excitation energies in neutron-deficient lead, and polonium isotopes. At prolate deformations, attention has been paid to the systematic prediction of high- $K$  states along the  $N = 102$  and  $104$  isotonic chains. Three high- $K$  states, namely,  $K^\pi = 7^-$ ,  $6^-$ , and  $6^+$  with  $\nu\{7/2^+[633], 7/2^-[514]\}$ ,  $\nu\{7/2^+[633], 5/2^-[512]\}$ , and  $\nu\{7/2^-[514], 5/2^-[512]\}$  configurations, respectively, have been found. Good agreements between calculations and

available data have been obtained. The high- $K$  states open up new possibilities for the study of the shape-coexistence phenomenon in this mass region. Low excitation energies, large  $K$ -values as well as rigid axially deformed shapes as compared to their ground states provide favorable conditions for the formation of isomers. The nucleus,  $^{186}\text{Pb}$ , is calculated to have high- $K$  isomers with distinct shapes (*oblate* and *prolate*) which coexist at similar excitation energies. It is remarkable that the oblate  $10^-$  states with the two-proton configuration  $\pi\{13/2^+[606], 7/2^-[514]\}$  are predicted to have significantly lower energies than other two-quasiparticle high- $K$  states in the polonium isotopes. This would indicate long-lived isomers existing in the neutron-deficient polonium isotopes, and a corresponding experimental search is needed.

## V. ACKNOWLEDGMENTS

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