Probing the gateway to superheavy nuclei in cranked relativistic Hartree-Bogoliubov theory

A. V. Afanasjev[1][*][†], T. L. Khoo[*], S. Frauendorf[†], G. A. Lalazissis[**] and I. Ahmad[*]

[*]*Physics Division, Argonne National Laboratory, Argonne, IL 60439, USA*
[†]*Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA*
[**]*Department of Theoretical Physics, Aristotle University of Thessaloniki, GR54124, Thessaloniki, Greece*

Abstract. The cranked relativistic Hartree+Bogoliubov theory has been applied for a systematic study of the nuclei around ^{254}No, the heaviest nuclei for which detailed spectroscopic data are available. The deformation, rotational response, pairing correlations, quasi-particle and other properties of these nuclei have been studied with different relativistic mean field (RMF) parametrizations. For the first time, the quasi-particle spectra of odd deformed nuclei have been calculated in a fully self-consistent way within the framework of the RMF theory. The energies of the spherical subshells, from which active deformed states of these nuclei emerge, are described with an accuracy better than 0.5 MeV for most of the subshells with the NL1 and NL3 parametrizations. However, for a few subshells the discrepancy reach 0.7-1.0 MeV. The implications of these results for the study of superheavy nuclei are discussed.

INTRODUCTION

The possible existence of shell-stabilized superheavy nuclei, predicted with realistic nuclear potentials [1, 2, 3] and the macroscopic-microscopic (MM) method [4, 5, 6], has been a driving force behind experimental and theoretical efforts to investigate the superheavy nuclei. These investigations pose a number of experimental and theoretical challenges. On the theoretical side, no consensus has been achieved on the question of what are the magic shell gaps in superheavy nuclei. The situation is illustrated in Table 1, where the predictions of different models are summarized.

The accuracy of predictions of spherical shell closures depends sensitively on the accuracy of describing the single-particle energies, which becomes especially important for superheavy nuclei, where the level density is very high. Variations in single-particle energy of $1-1.5$ MeV yield spherical shell gaps at different particle numbers, which restricts the reliability in extrapolating to an unknown region.

The MM method describes the single-particle energies rather well in known regions. This is due to the fact that the experimental data on single-particle states are used directly in the parametrization of the single-particle potential. However, the extrapolation of the single-particle potential may be much less reliable since it is not determined self-consistently. For example, microscopic models predict that the appearance of shell closures in superheavy nuclei is influenced by a central depression of the nuclear density distribution [7, 8]. This effect is not treated in a self-consistent way in current MM models.

Although the nucleonic potential is defined in self-consistent approaches, such as Skyrme Hartree-Fock (SHF) and relativistic mean field (RMF) theory, in a fully self-consistent way, this does not guarantee that single-particle degrees of freedom are accurately described. This is especially true because the parameters of the Skyrme forces and RMF Lagrangians were fitted mostly to bulk properties, and the accuracy of the description of the single-particle energies is poorly known. Compared with the MM method, self-consistent calculations have been confronted with experiment to a lesser degree and for a smaller number of physical observables (mainly binding energies and quantities related to their derivatives). For many parametrizations, even the reliability of describing conventional nuclei is poorly known.

In order to fill this gap in our knowledge, the cranked relativistic Hartree+Bogoliubov (CRHB) theory [16, 17] has

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[1] on leave of absence from the Laboratory of Radiation Physics, Institute of Solid State Physics, University of Latvia, LV 2169 Salaspils, Miera str. 31, Latvia

TABLE 1. Predicted magic spherical shell gaps for superheavy nuclei.

Method	Proton shell gap	Neutron shell gap	Potential in the MM method	References
MM	114	184	Nilsson	[5]
			Woods-Saxon	[4, 9, 10]
			folded Yukawa	[11]
Skyrme	126*	184		[10, 12, 7]
Gogny	120/126	172/184		[13]
RMF	120†	172		[12, 7]

* Only the values appearing in most of the parametrizations are quoted. Some Skyrme forces indicate $Z = 114$ (SkM*) and $Z = 120$ (SkI3) as proton shell closures, while some (for example, SkP) predict no doubly magic superheavy nuclei at all.

† The NLSH (NLRA1) parametrizations of the RMF Lagrangian give (also) $Z = 114$ and $N = 184$ as shell closures [14, 15], but since they give a poor description of quasiparticle spectra in the deformed $A \sim 250$ mass region, we consider these predictions less reliable than those obtained with other RMF sets.

been applied for a systematic study of the nuclei around ^{254}No, the heaviest elements for which detailed spectroscopic data are available. The deformations, rotational response, pair correlations, quasiparticle spectra, shell structure and the two-nucleon separation energies have been studied. The goal was to see how well the theory describes the experimental data and how this description depends on the RMF parametrization. The details of this study will be reported in a forthcoming manuscript [18].

In the present contribution, we mainly concentrate on the results having implications for the study of superheavy nuclei. Particular attention is paid to the comparison of experimental and calculated quasiparticle spectra in deformed nuclei and, based on that, how one can estimate the accuracy of the calculated energies of spherical subshells. One can then (i) judge which RMF parametrizations provide best description of single-particle energies and thus are best suited for the study of superheavy nuclei and (ii) assess how the RMF predictions for superheavy nuclei are modified if empirical shifts for the energies of spherical subshells, deduced from the study of deformed nuclei, are taken into account.

SHELL STRUCTURE IN THE DEFORMED $A \sim 250$ MASS REGION.

The stability of the superheavy elements is due to a 'shell gap', i. e. a region of low level density in the single-particle spectrum. The quantity $\delta_{2n}(Z,N)$ related to the derivative of the separation energy is a sensitive indicator of the localization of the shell gaps. For the neutrons (and similarly for the protons) it is defined as

$$\begin{aligned} \delta_{2n}(Z,N) &= S_{2n}(Z,N) - S_{2n}(Z,N+2) = \\ &= -B(Z,N-2) + 2B(Z,N) - B(Z,N+2) \end{aligned} \tag{1}$$

where $B(N,Z)$ is the binding energy.

We study the accuracy of the description of shell structure with different parametrizations of the RMF Lagrangian in the deformed $A \sim 250$ mass region. Fig. 1 compares experimental and calculated $\delta_{2p}(Z,N)$ quantities for the $N = 152$ isotone chain. The experimental data shows a shell gap at $Z = 100$. Only NLSH describes the position of this gap and the $\delta_{2p}(Z,N)$ values agree very well. However, the quasi-particle spectra in Ref. [18] reveal that this gap lies between the wrong bunches of single-particle states. Calculations with NLSH also indicate a gap at $Z = 108$, which has not been observed so far. NL-RA1 does not show any deformed gap for $92 \leq Z \leq 108$. NL3, NL1 and NL-Z give a shell gap at $Z = 104$, in contradiction with experiment.

For the Fm $(Z = 100)$ isotope chain, NL3 and NL-RA1 (NL1 and NL-Z) produce a gap at $N = 148$ ($N = 148, 150$) instead of at $N = 152$ as seen in experiment; NLSH does not show a clear gap. Many effective interactions not specifically fitted to the actinide region encounter similar problems in the description of deformed shell gaps in the $A \sim 250$ mass region; see for example Ref. [19]).

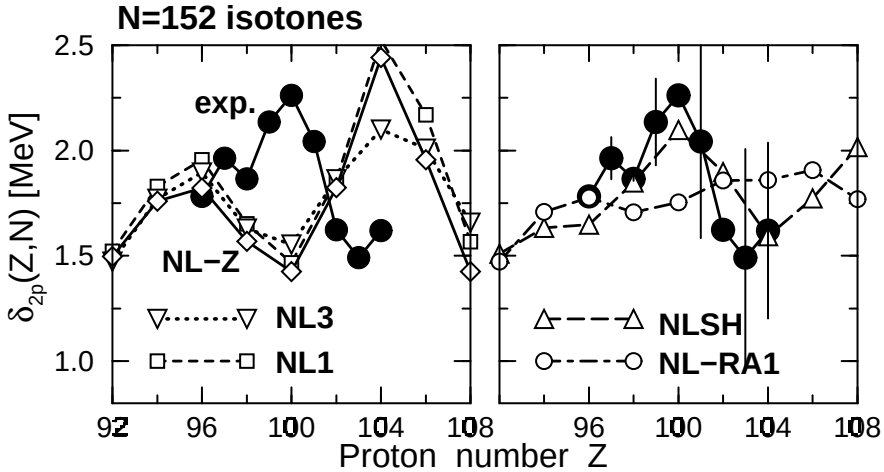

FIGURE 1. The $\delta_{2p}(Z,N)$ quantity for the chain of $N = 152$ isotones obtained in the CRHB+LN calculations with indicated RMF parametrizations. Solid circles are used for experimental data, while open symbols for theoretical results. The experimental error bars are shown in right panel.

QUASIPARTICLE SPECTRA IN ODD-MASS $A \sim 250$ NUCLEI

The fact that the experimental quadrupole deformations of the nuclei in this mass region are very well described in the CRHB+LN calculations (see Ref. [18] for details) strongly suggests that the discrepancies between experimental and calculated $\delta_{2p}(Z,N)$ are due to inaccurate deformed single-particle states with present RMF parametrizations. This, in turn, is due to errors in the positions of spherical subshells from which the deformed states emerge. Thus, the investigation of the single-particle states in the $A \sim 250$ deformed mass region can shed additional light on the reliability of the predictions of RMF theory on the energies of spherical subshells responsible for 'magic' numbers in superheavy nuclei. This is because several deformed single-particle states experimentally observed in odd nuclei of this mass region (see Table 2) originate from these subshells.

A proper description of odd nuclei implies the loss of the time-reversal symmetry of the mean-field, which is broken by the unpaired nucleon. The BCS approximation has to be replaced by the Hartree-(Fock-)Bogoliubov method, with time-odd mean fields taken into account. The breaking of time-reversal symmetry leads to the loss of the double degeneracy (Kramer's degeneracy) of the quasiparticle states. This requires the use of the signature or simplex basis in numerical calculations, thus doubling the computing task. Furthermore, the breaking of the time-reversal symmetry leads to nucleonic currents, which causes *nuclear magnetism* [20]. The CRHB(+LN) theory takes all these effects into account and thus address for the first time the question of a fully self-consistent description of quasiparticle states in the framework of the RMF theory.

The CRHB code [17] has been extended to describe odd and odd-odd nuclei. The blocked orbital can be specified either by its dominant main oscillator quantum number N or by the dominant Ω quantum number (Ω is the projection of the total angular momentum on the symmetry axis) of the wave function, or by combination of both. In addition, it can be specified by the particle or hole nature of the blocked orbital.

Experimental and calculated spectra of ^{249}Bk and ^{251}Cf are compared in Fig. 2. This is the first ever direct comparison between experiment and theoretical quasiparticle spectra obtained for deformed nuclei within the framework of the RMF theory. The CRHB calculations have been performed with D1S force [21] in the particle-particle channel and with NL1 and NL3 parametrizations [22, 23] of the RMF Lagrangian. Since the results are discussed in detail in Ref. [18], only main features will be outlined below.

Although the same set of quasiparticle states as in experiment appears, the calculated spectra are less dense. This is related to the effective mass (Lorentz mass in the notation of Ref. [24]) of the nucleons at the Fermi surface $m^*(k_F)/m$. While the experimental density of the quasiparticle levels corresponds to $m^*(k_F)/m$ close to one, the low effective mass $m^*(k_F)/m \approx 0.66$ of the RMF theory [7] leads to a stretching of the energy scale. It has been demonstrated for spherical nuclei that the particle-vibration coupling brings the average level density in closer agreement with experiment [28]. In a similar way, the particle-vibration coupling leads to a compression of the quasi-particle spectra in

TABLE 2. Spherical subshells active in superheavy nuclei and their deformed counterparts active in the $A \sim 250$ mass region. The left column shows the spherical subshells active in the vicinity of the "magic" spherical gaps $(Z = 120, N = 172)$. Their ordering is given according to the RMF calculations with the NL3 parametrizations in the $^{292}_{172}120$ system (see Fig. 3). Although the gaps depend on the specific RMF parametrization, the same set of spherical subshells is active with other parametrizations (see, for example, Fig. 4 in Ref. [7]). The right column shows the deformed quasiparticle states observed in $^{249}_{97}\mathrm{Bk}_{1K2}$ [25] and $^{249,251}_{98}\mathrm{Cf}_{1K1,1K2}$ [26, 27]. The bold style is used for the states which might be observed when either proton or neutron number is increased by ≈ 10 as compared with these nuclei. The symbols 'N/A' (not accessible) are for the deformed states which typically increase their energy with increasing deformation and thus are not likely to be seen experimentally.

Proton states Spherical subshell	Deformed state	Neutron states Spherical subshell	Deformed state
		$\nu 1k_{17/2}$	**ν [880]1/2**
$\pi 1j_{15/2}$	**π [770]1/2**	$\nu 2h_{11/2}$	**ν [750]1/2**
$\pi 3p_{1/2}$	N/A	$\nu 1j_{13/2}$	ν[761]1/2
$\pi 3p_{3/2}$	N/A	$N = 184$	
$\pi 1i_{11/2}$	**π [651]1/2**	$\nu 4s_{1/2}$	N/A
$Z = 120$		$\nu 3d_{5/2}$	ν[620]1/2
$\pi 2f_{5/2}$	π[521]1/2	$\nu 3d_{3/2}$	N/A
$\pi 2f_{7/2}$	π[521]3/2, π[530]1/2	$N = 172$	
$\pi 1i_{13/2}$	π[642]5/2, π[633]7/2, π[624]9/2	$\nu 2g_{7/2}$	ν[622]3/2
$\pi 3s_{1/2}$	π[400]1/2	$\nu 2g_{9/2}$	ν[622]5/2, ν[613]7/2, ν[604]9/2
$\pi 1h_{9/2}$	π[514]7/2	$\nu 1j_{15/2}$	ν[734]9/2, ν[725]11/2
		$\nu 1i_{11/2}$	ν[615]9/2, ν[624]7/2

deformed nuclei [29]. The surface vibrations are less collective in deformed nuclei than in spherical ones because they are more fragmented [30, 31]. As a consequence, the corrections to the energies of quasiparticle states in odd nuclei due to particle-vibration coupling are less state-dependent in deformed nuclei. Hence the comparison between experimental and mean field single-particle states is less ambiguous in deformed nuclei as compared with spherical ones [28, 31], at least at low excitation energies, where vibrational admixtures to the wave functions are small. Assuming for an estimate that the effective mass just stretches the energy scale, one can show that the uncertainty of our estimate for the spherical subshell energies derived from the energies of deformed states can be kept below 300 keV.

Fig. 2 shows that the calculated energies of a number of states are rather close to experiment. On the other hand, the energies of some states and their relative positions deviate substantially from experiment. For example, only NL1 gives the correct ground state $\nu[620]1/2$ in ^{251}Cf, whereas NL3 gives the $\nu[615]9/2$. Detailed analysis shows that the discrepancies between experiment and calculations can be traced back to energies of spherical subshells from which deformed states emerge. This allows us to define 'empirical shifts' to the energies of spherical subshells which, if incorporated, will correct the discrepancies between calculations and experiment seen for deformed quasiparticle states. These 'empirical shifts' are shown in Fig. 3 as the energy difference between self-consistent and corrected energies of specific subshells. It is important to note that these corrections lead to a deformed $N = 152$ shell gap and to a larger $Z = 100$ shell gap, thus improving the description of the shell structure (for example, the $\Delta_{2p,n}(Z,N)$ quantities) in the deformed $A \sim 250$ mass region.

IMPLICATIONS FOR THE STUDY OF SUPERHEAVY NUCLEI

In the NL1 and NL3 parametrizations, the energies of the spherical subshells, from which the deformed states in the vicinity of the Fermi level of the $A \sim 250$ nuclei emerge, are described with an accuracy better than 0.5 MeV for most of the subshells (see Fig. 3 where 'empirical shifts', i.e. corrections, for single-particle energies are indicated). The discrepancies (in the range of 0.6-1.0 MeV) are larger for the $\pi 1h_{9/2}$ (NL3, NL1), $\nu 1i_{11/2}$ (NL3), $\nu 1j_{15/2}$ (NL1) and $\nu 2g_{9/2}$ (NL3) spherical subshells. Considering that the RMF parametrizations were fitted only to bulk properties of spherical nuclei this level of agreement is good. The NL-Z [35] force provides comparable level of accuracy.

In contrast, the accuracy of the description of single-particle states is unsatisfactory in the NLSH and NL-RA1 parametrizations, where 'empirical shifts' to the energies of some spherical subshells are much larger than in NL1 and NL3. NL-SH and NL-RA1 are the only RMF sets indicating $Z = 114$ as a magic proton number [14, 15]. In the light

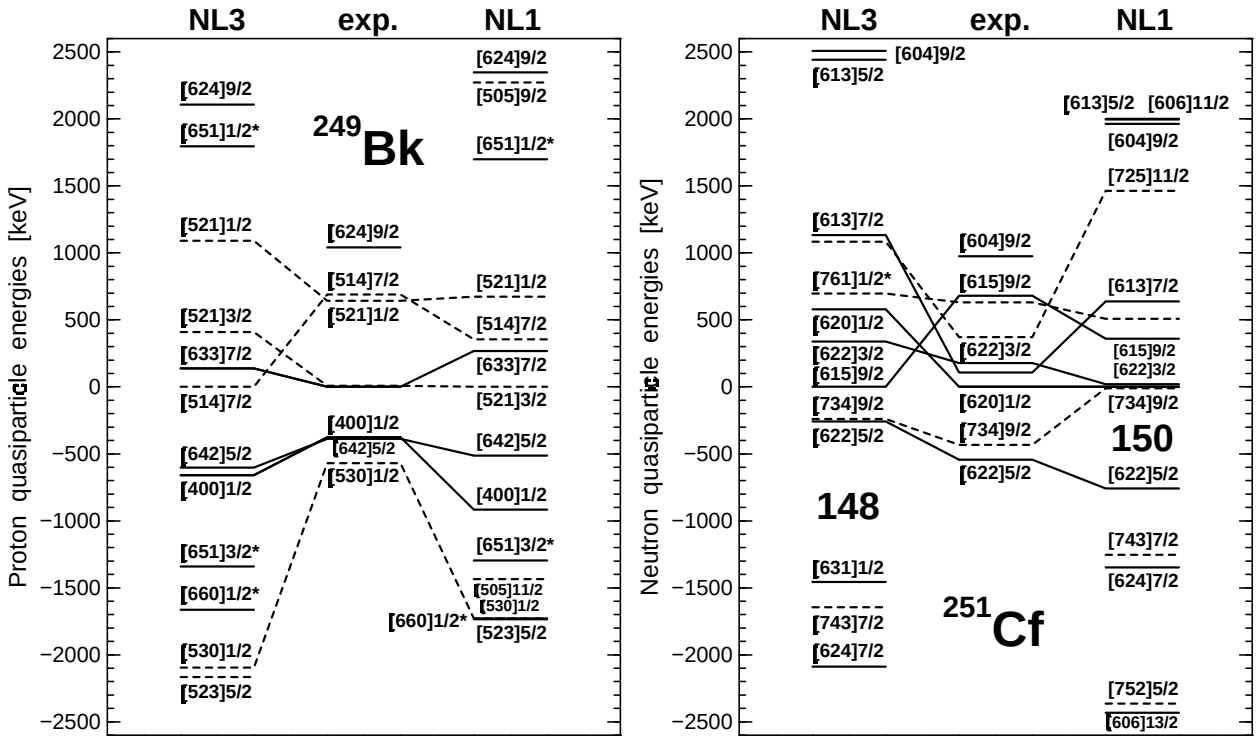

FIGURE 2. Experimental and theoretical quasiparticle energies of neutron states in ^{249}Cf. Positive and negative energies are used for particle and hole states, respectively. The experimental data are taken from Ref. [26]. Solid and dashed lines are used for positive and negative parity states, respectively. The symbols 'NL3' and 'NL1' indicate the RMF parametrization. In each calculational scheme, attempts were made to obtain solutions for every state shown in figure. The absence of a state indicates that convergence was not reached.

of present results, this prediction should be treated with a considerable caution.

The spectra of spherical magic superheavy nuclei are not modified much with empirical shifts (see Fig. 3 for the calculated and corrected single-particle spectra of a $^{292}_{172}$120 nucleus). Such a study relies on the assumption that these corrections (which essentially apply to the l-shells from which spin-orbit partner j-shells ($j = l \pm 1/2$) emerge) should be similar in deformed $A \sim 250$ mass region and in superheavy nuclei. The corrected spectra from the NL1 and NL3 calculations are very similar with minor differences coming from the limited amount of information on quasiparticle states used in an analysis. More systematic study of quasiparticle states in deformed nuclei are required to determine these corrections more precisely.

Let us consider the calculations for the $Z = 120, N = 172$ nucleus. The corrected spectra still suggest that $N = 172$ and $N = 184$ are candidates for magic neutron numbers in superheavy nuclei. The position of the $\nu 1a_{1/2}$ spherical subshell and the spin-orbit splitting of the $3d_{5/2}$ and $3d_{3/2}$ subshells will decide which of these numbers (or both of them) is (are) magic. The corrected proton spectra indicate that the $Z = 120$ gap is large whereas the $Z = 114$ gap is small. Hence, on the basis of the present investigation we predict that $Z = 120$ is the magic proton number. This conclusion is based on the assumption that the NL1 and NL3 sets predict the position of the $\pi 1i_{11/2}$ and $\pi 3p_{1/2,3/2}$ subshells within 1 MeV error. The positions of $\pi 1j_{15/2}$ and $\pi 2g_{9/2}$ seems less critical, because they are located well above this group of states both in Skyrme and RMF calculations [7]. It seems possible to obtain information about the location of the $\pi 1i_{11/2}$ subshell, which may have been observed through its deformed state ($\pi[651]1/2$) in superdeformed rotational bands of Bi-isotopes [32, 33]. An CRHB analysis may provide this critical information.

The Nilsson diagrams given, for example, in Figs. 3 and 4 of Ref. [34] suggest that spectroscopic studies of deformed odd nuclei with proton and neutron numbers up to $Z \approx 108$ and $N \approx 164$ may lead to observation of the deformed states with $\Omega = 1/2$, emerging from the $\pi 1i_{11/2}$ and $\pi 1j_{15/2}$ spherical subshells located above the $Z = 120$ shell gap and from $\nu 1k_{17/2}$ and either $\nu 2h_{11/2}$ or $\nu 1j_{15/2}$ subshells located above the $N = 184$ shell gap. This will further constrain microscopic models and effective interactions.

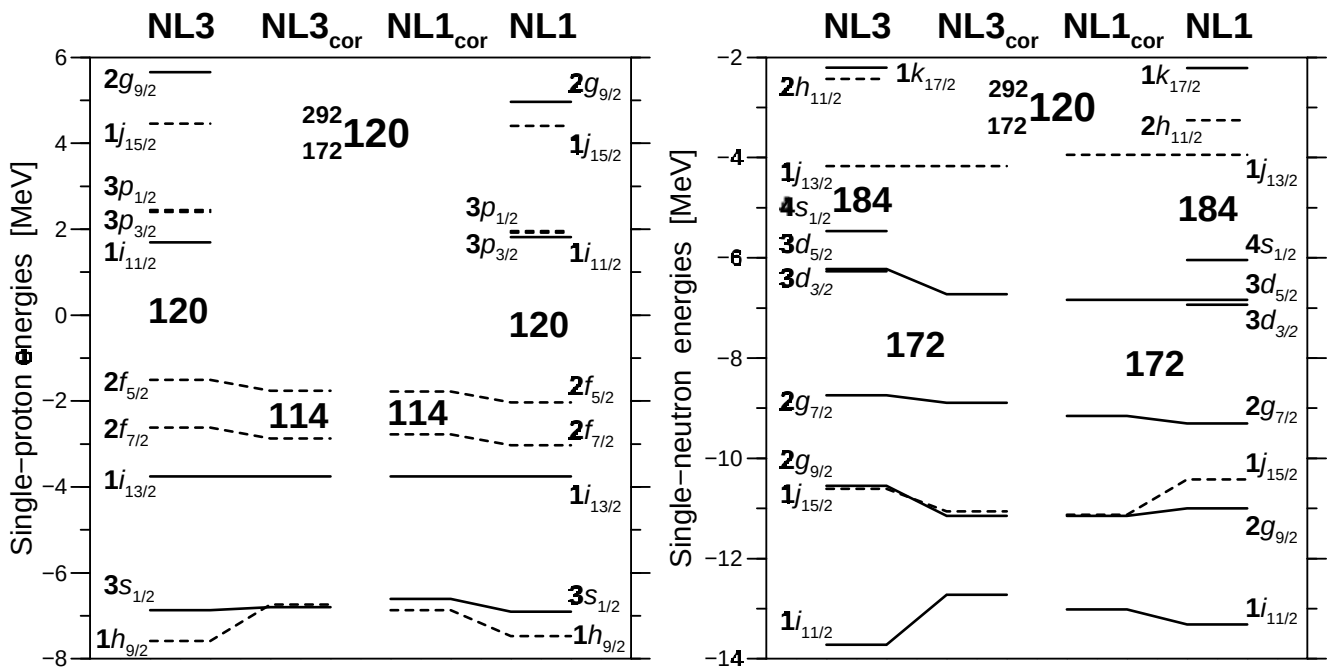

FIGURE 3. Proton and neutron single-particle states in a $^{292}_{172}120$ nucleus. Columns 'NL3' and 'NL1' show the states obtained in the RMF calculations at spherical shape with the indicated parametrizations. For proton system, the energy of the $1i_{13/2}$ state in the NL1 parametrization is set to be equal to the one in NL3, which means that the energies of all states in NL1 (last column) are increased by 0.78 MeV. For neutron sysytem, the energies of all states obtained with the NL1 parametrization (last column) are increased by 0.76 MeV in order to have the same energies of the $2g_{9/2}$ states in the second and third columns. The columns 'NL3$_{cor}$' and 'NL1$_{cor}$' show how the spectra are modified if empirical shifts were introduced based on discrepancies between calculations and experiment for quasiparticle spectra in ^{249}Bk and ^{249,251}Cf. Solid and dashed lines are used for positive and negative parity states. Spherical gaps at $Z = 114, Z = 120$ and at $N = 172, N = 184$ are indicated.

No information on low-j states, such as $\pi 3g_{9/2}$, $\pi 3p_{1/2}$, $\nu 3d_{5/2}$ and $\nu 1s_{1/2}$, which decide whether $Z = 120$ or $Z = 126$ and $N = 172$ or $N = 184$ are magic numbers in microscopic theories (see Refs. [7, 36] and references quoted therein) will come from the study of deformed nuclei (see Table 2).

The measured and calculated energies of the single-particle states at normal deformation provide constraints on the spherical shell gaps of superheavy nuclei. In particular, the small splitting between the $\pi[521]1/2$ and $\pi[521]3/2$ deformed states, from the $\pi 2f_{5/2}$ and $\pi 2f_{7/2}$ spherical subshells that straddle proton number 114, suggests that the $Z = 114$ shell gap is not large. More systematic studies of the splitting between the $\pi[521]1/2$ and $\pi[521]3/2$ deformed states may provide more stringent information on whether a shell gap exists at $Z = 114$.

CONCLUSIONS

The cranked relativistic Hartree+Bogoliubov theory has been applied for a systematic study of the nuclei around ^{254}No, the heaviest nuclei for which detailed spectroscopic data are available. The deformations, rotational response, pair correlations, quasiparticle spectra, shell structure and two-nucleon separation energies have been studied. The part of this study devoted to the investigation of quasiparticle states and its implications for the study of superheavy nuclei is presented in this contribution. It is concluded that the energies of the spherical subshells, from which active deformed states of these nuclei emerge, are described with an accuracy better than 0.5 MeV for most of the subshells with the NL1 and NL3 parametrizations. However, for a few subshells the discrepancies reach 0.7-1.0 MeV. Amongst the investigated RMF sets, NL1, NL3 and NL-Z provide best description of single-particle states so they are recommended for the study of superheavy nuclei. The corresponding self-consistent calculations predict as candidates for magic numbers $N = 172$ and $N = 184$ for neutrons and $Z = 120$ for protons. No significant shell gap is found at $Z = 114$.

These conclusions take into account the possible shifts of spherical subshells that are suggested by the discrepancies between calculations and experiment for deformed states in the $A \sim 250$ mass region found in our analysis.

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