Ground-state properties and spins of the odd $Z=N+1$ nuclei ^{61}Ga$-^{97}$In

S. K. Patra, M. Del Estal, M. Centelles, and X. Viñas
Departament d'Estructura i Constituents de la Matèria, Facultat de Física, Universitat de Barcelona, Diagonal 647, E-08028 Barcelona, Spain

(Received 7 August 2000; revised manuscript received 18 October 2000; published 22 January 2001)

Binding energies, quadrupole deformation parameters, spins, and parities of the neutron-deficient odd $Z=N+1$ nuclei in the $A\sim 80$ region are calculated in the relativistic mean field approximation. The ground-state and low-lying configurations of the recently observed ^{77}Y, ^{79}Zr, and ^{83}Mo nuclei are analyzed. The calculated results are compared with other theoretical predictions.

DOI: 10.1103/PhysRevC.63.024311 PACS number(s): 21.10.Dr, 21.30.Fe, 21.60.Jz, 27.50.+e

I. INTRODUCTION

Beyond $Z\approx 20$ the stability of nuclei requires additional neutrons because of the Coulomb repulsion among protons and the most stable nuclei are those with $N>Z$ [1]. However, a large number of nuclei are possible whose N and Z numbers differ considerably from this line of β stability. The properties of light systems near the limits of stability of proton/neutron-rich nuclei have attracted considerable experimental and theoretical attention [2–7]. The availability of radioactive beams in various laboratories will likely provide much intriguing experimental information on the structure and reactions of these nuclei. The discovery of new isotopes [3] has opened a new path of nucleosynthesis by rapid proton capture [5]. Similarly, the discovery of new neutron-rich nuclei near the drip line is important to understand the rapid neutron capture process in accreting stellar systems [8].

In the region of $A\sim 80$, nuclei with nearly equal numbers of protons and neutrons are of fundamental interest and can now be studied using radioactive beams [9]. The structural properties of these nuclei are strongly determined by deformed shell gaps in the nuclear single-particle potential [10]. The deformation properties of these nuclei change dramatically by addition or removal of one or two nucleons [11,12]. The nucleon numbers (N or Z) 36 and 38 have been identified with highly deformed oblate [13] and prolate [11,14] shell gaps, respectively. Recently, the very neutron-deficient $Z=N+1$ ($T_z=-1/2$) nuclei ^{77}Y, ^{79}Zr, and ^{83}Mo have been observed [4]. The deformation properties of these nuclei and the energies of the last occupied single-particle state of the odd proton are very crucial from stability and astrophysical points of view.

Wallace and Woosley [15] have conjectured a rapid proton capture process in accreting matter that provides a way for synthesizing very neutron-deficient nuclei close to the proton drip line in the $A\approx 60-80$ region [16]. In this case the asymmetry energy is relatively unimportant because of the near equality of Z and N. The existence of these new highly neutron-deficient isotopes stems from a delicate balance between the attractive nuclear force and the repulsive electrostatic force in atomic nuclei. On average, the nuclear force is attractive between a proton and a neutron and less attractive between two protons or two neutrons. Thus there is a limit to the excess number of protons over neutrons, or vice versa, one can have in a nucleus. This situation is further aggravated by the electromagnetic Coulomb repulsion among protons which strives to break the nucleus apart. The limits to the number of protons/neutrons are known as the proton/neutron drip lines. Due to the increasing importance from both the experimental and theoretical sides of the mass region $A\sim 80$, it is worthwhile to investigate the ground-state properties and spin of these nuclei, which is the prime aim of this work.

The article is organized as follows. Section II is devoted to some basic points of the relativistic mean field (RMF) calculations. We present our results obtained by various RMF parameter sets in Sec. III. Finally, the summary and concluding remarks are given in Sec. IV.

II. CALCULATIONS

We shall calculate the deformation properties and the single-particle energies and spins of the last occupied proton states for odd $Z=N+1$ systems using an axially deformed relativistic mean field (RMF) formalism [17,18]. From the relativistic Lagrangian we get the field equations for the nucleons and the mesons. These equations are solved by expanding the upper and lower components of the Dirac spinors and the boson fields in a deformed oscillator basis with an initial deformation β_0. $N_{\mathrm{F}}=12$ and $N_{\mathrm{B}}=20$ oscillator shells are used as the expansion basis for the fermion and boson fields [17]. The set of coupled equations is solved numerically by a self-consistent iteration method. The center-of-mass motion is estimated by the usual harmonic oscillator formula. We evaluate the one-proton separation energy (S_{p}) from the binding energies of the two neighboring nuclei with Z and $Z-1$ protons [1]:

$$S_{\mathrm{p}}(N,Z)=B(N,Z)-B(N,Z-1), \tag{1}$$

where $B(N,Z)$ is the binding energy for neutron number N and proton number Z. The quadrupole deformation parameter β_2 is evaluated from the resulting quadrupole moment [17].

Our calculations will be performed with the NL1 [19], NL-SH [20], TM1 [21], and NL3 [22] parameter sets. The predictive power of these parametrizations is well known and some examples can be found, e.g., in Ref. [23] and references quoted therein. It is to be noted that the RMF parameter sets are determined by fitting nuclear matter properties, neutron-proton asymmetry energies, root-mean-square radii and binding energies of some spherical nuclei. Then, there is no further adjustment to be made in the parameters of the Lagrangian. The NL1 set was preferred in early calculations [24]. However, it does not describe well the neutron skin thickness of neutron-rich nuclei due to a very large asymmetry energy, and predicts relatively large quadrupole deformations near the neutron drip line [20]. To cure these deficiencies, data on neutron radii were included in the fit of the parameters of the NL-SH interaction. An interesting feature of the TM1 parametrization [21] is that in this set the sign of the quartic scalar self-coupling is positive (contrary to NL1, NL-SH, and NL3). This could be achieved by introducing a quartic self-interaction of the vector field in the effective force. In general the quality of the results reproduced by TM1 is not superior to the standard nonlinear sets and it has not been much used in the literature. The relatively new parameter set NL3 is considered to be very successful and there is confidence that it can be used fruitfully for the investigation of new regions of nuclear stability.

The calculation of odd-even and odd-odd nuclei in an axially deformed basis is a tough task in the RMF model. To take care of the lone odd nucleon one has to violate time-reversal symmetry in the mean field. In the present study only the timelike components V_0, b_0, and A_0 of the ω, ρ, and photon fields are retained. The space components of these fields (which are odd under time reversal and parity) are neglected. They are important in the determination of properties like magnetic moments [25], but have a very small effect on bulk properties like binding energies or deformations and can be neglected to a good approximation [30]. In our calculation of odd nuclei we employ the blocking approximation, which restores the time-reversal symmetry. In this approach one pair of conjugate states $\pm m$ is taken out of the pairing scheme. The odd particle stays in one of these states and its corresponding conjugate state remains empty. In general one has to block in turn different states around the Fermi level to find the one which gives the lowest energy configuration of the odd nucleus. In odd-odd nuclei (which will be needed in our calculations of separation energies) we have blocked both the odd proton and the odd neutron.

For known nuclei close to or not too far from the stability line, the Bardeen-Cooper-Schrieffer (BCS) approach provides a reasonably good description of the pairing properties. However, in going to nuclei in the vicinity of the drip lines the coupling to the continuum becomes important. It has been shown that the self-consistent treatment of the BCS approximation breaks down when coupling between bound states and states in the continuum takes place [26]. For most of the very neutron-deficient nuclei of our study odd-even mass differences are not measured and little is known about the precise effect of the pairing interaction. It is expected that for odd-even nuclei the effects of pairing are considerably decreased [1]. In the present investigation we have chosen to use a BCS formalism with a small constant pairing strength, namely $\Delta_n = \Delta_p = 0.5$ MeV. This value of the gaps contributes very little to the total binding (unless the pairing gap is varied considerably our results remain unchanged). This type of prescription has already been adopted in the past [27].

Certainly, for properties like radii of halo nuclei that sensitively depend on the spatial extension of the nucleon densities a more proper treatment of the continuum could be crucial, e.g., by means of the relativistic Hartree-plus-Bogoliubov (RHB) approach [28–30]. In this model the wave functions of the occupied quasiparticle states have the correct asymptotic behavior. Results of RHB and RMF-BCS calculations have been compared in Ref. [7] for neutron-rich nuclei in the deformed $N=28$ region. The two models have been found to predict almost identical binding energies and similar quadrupole deformations, though they differ significantly in the calculated rms radii (they turn out to be larger in the RMF-BCS model). A recent RHB study of deformed odd-Z proton emitters in the $53 \leqslant Z \leqslant 69$ region using the NL3 set has been published in Ref. [30]. For the lightest isotopes ^{107}I, ^{108}I, and ^{109}I reported in Table I of that work, the odd valence proton occupies a $[422]3/2^+$ Nilsson orbital (see below for notation) and the ground-state quadrupole deformations are $\beta_2 = 0.15$, 0.16, and 0.16, respectively. For comparison we have performed the calculations with our model and find the same $[422]3/2^+$ orbital for the three isotopes and deformations $\beta_2 = 0.17$, 0.18, and 0.19, respectively, in rather good agreement with the more sophisticated RHB method.

III. RESULTS AND DISCUSSION

We now discuss the results of our RMF calculations for the neutron-deficient nuclei ^{61}Ga, ^{65}As, ^{69}Br, ^{73}Rb, ^{77}Y, ^{81}Nb, ^{85}Tc, ^{89}Rh, ^{93}Ag, and ^{97}In, i.e., the odd-proton, $T_z = -1/2$ nuclei in the interval $31 \leqslant Z \leqslant 49$ with $Z = N+1$. For a given nucleus the solution with the largest binding energy corresponds to the ground-state configuration and the other solutions are the excited intrinsic states. In the present calculations we find two or three different solutions for most of the isotopes, each solution differing in the deformation from the others. All the solutions are often close in energy with one another, and sometimes they are nearly degenerate. In the case of finding almost degeneracy there is some uncertainty in the determination of the ground-state solution: a change in the inputs of the calculation (e.g., the parameter $\hbar\omega = 41 A^{-1/3}$ MeV) may alter the prediction for the ground-state shape. The low-lying excited solutions can be interpreted as solutions with coexisting shapes. The shape coexistence nature in the $A \sim 80$ region has been reported in Refs. [31,32].

In Tables I–III we present our RMF results for the binding energy and the quadrupole deformation parameter β_2. We also list the single-particle energy ϵ_p of the blocked state, occupied by the odd proton, as well as its Nilsson state labelings $[N n_3 \Lambda]\Omega^\pi$ (Ω^π being the spin and parity of the orbit; for spherical solutions we use spherical quantum numbers). For these odd-mass nuclei the spin of the odd nucleon is the resultant spin of the nucleus. In the tables we also display results of microscopic-macroscopic (MM) mass models for comparison. The values from the tabulation of Ref. [33], based on the finite-range droplet model and folded

TABLE I. RMF results for the binding energy (B), the quadrupole deformation parameter (β_2), and the single-particle energy ϵ_p and Nilsson orbit $[Nn_3\Lambda]\Omega^\pi$ of the state occupied by the odd proton are shown for the nuclei ^{61}Ga, ^{65}As, and ^{69}Br. Results of microscopic-macroscopic (MM) mass models are also given: MMa is from Ref. [33] and MMb is from Ref. [4]. The energies are in MeV.

	Set	ϵ_p	$[Nn_3\Lambda]\Omega^\pi$	β_2	B
^{61}Ga	NL1	−1.06	$[310]1/2^-$	0.21	513.7
		−2.17	$[301]1/2^-$	−0.13	511.6
	NL-SH	−0.91	$[312]3/2^-$	0.22	513.1
		−1.50	$[301]3/2^-$	−0.18	510.5
	TM1	−1.61	$[312]3/2^-$	0.23	512.0
		−2.16	$[301]3/2^-$	−0.20	509.9
	NL3	−0.89	$[312]3/2^-$	0.23	511.3
		−1.88	$[301]3/2^-$	−0.19	508.4
	MMa		$1/2^-$	0.21	
^{65}As	NL1	−2.21	$[312]3/2^-$	0.24	542.7
		−2.99	$[301]1/2^-$	−0.25	542.4
	NL-SH	−1.39	$[310]1/2^-$	0.23	541.9
		−2.23	$[301]1/2^-$	−0.23	540.9
	TM1	−1.95	$[310]1/2^-$	0.24	543.1
		−2.78	$[301]1/2^-$	−0.25	542.5
	NL3	−1.95	$[310]1/2^-$	0.24	540.2
		−2.56	$[301]1/2^-$	−0.24	539.9
	MMa		$3/2^-$	0.23	
^{69}Br	NL1	−0.94	$[404]9/2^+$	−0.29	575.5
		−0.78	$[301]3/2^-$	0.21	574.2
	NL-SH	−1.52	$[404]9/2^+$	−0.28	573.1
		−0.35	$[431]1/2^+$	0.28	571.6
	TM1	−1.21	$[404]9/2^+$	−0.29	575.7
		−0.44	$[303]5/2^-$	0.22	574.3
	NL3	−1.23	$[404]9/2^+$	−0.29	572.5
		−0.20	$[431]1/2^+$	0.28	570.9
	MMa		$9/2^+$	−0.32	
	MMb		$[404]9/2^+$	−0.25	

TABLE II. Same as Table I for ^{73}Rb, ^{77}Y, and ^{81}Nb.

	Set	ϵ_p	$[Nn_3\Lambda]\Omega^\pi$	β_2	B
^{73}Rb	NL1	−0.74	$[413]7/2^+$	−0.35	605.0
		−2.23	$[431]3/2^+$	0.42	604.1
	NL-SH	−1.05	$[413]7/2^+$	−0.34	604.7
		−2.34	$[431]3/2^+$	0.41	602.6
	TM1	−0.73	$[404]7/2^+$	−0.35	605.8
		−1.83	$[431]3/2^+$	0.42	603.4
	NL3	−0.87	$[413]7/2^+$	−0.35	602.9
		−2.16	$[431]3/2^+$	0.42	601.4
	MMa		$3/2^+$	0.37	
	MMb		$[312]3/2^-$	0.42	
^{77}Y	NL1	−1.01	$[422]5/2^+$	0.49	638.0
		−1.35	$[330]1/2^-$	−0.08	637.7
	NL-SH	−1.22	$[422]5/2^+$	0.47	636.9
		−1.15	$[404]9/2^+$	−0.14	631.4
		−1.29	$p_{1/2}$	0.00	630.2
	TM1	−0.67	$[404]9/2^+$	−0.14	636.9
		−1.89	$p_{1/2}$	0.00	636.4
		−0.67	$[422]5/2^+$	0.49	635.7
	NL3	−1.00	$[422]5/2^+$	0.48	635.1
		−0.84	$[404]9/2^+$	−0.15	632.6
		−1.90	$p_{1/2}$	0.00	631.9
	MMa		$5/2^+$	0.42	
	MMb		$[422]5/2^+$	0.43	
^{81}Nb	NL1	0.04	$[404]9/2^+$	−0.02	670.6
		−1.25	$[413]7/2^+$	−0.21	668.1
		−0.42	$[431]1/2^+$	0.53	667.8
	NL-SH	−0.02	$[431]1/2^+$	0.52	667.1
		−1.63	$[413]7/2^+$	−0.20	663.8
		−0.43	$[404]9/2^+$	−0.02	660.4
	TM1	0.11	$[404]9/2^+$	−0.02	667.6
		−1.11	$[413]7/2^+$	−0.20	667.3
		−0.99	$[431]1/2^+$	0.55	664.9
	NL3	−0.26	$[431]1/2^+$	0.53	664.7
		−1.34	$[413]7/2^+$	−0.20	663.7
		−0.07	$[404]9/2^+$	−0.02	663.5
	MMa		$1/2^+$	0.46	
	MMb		$[431]1/2^+$	0.44	

Yukawa single-particle potential, will be labeled by MMa. The microscopic-macroscopic calculations described in Ref. [4] (mass formula plus Strutinsky correction) will be labeled by MMb.

The RMF calculations predict a moderate prolate and a moderate oblate solution for the ^{61}Ga, ^{65}As, and ^{69}Br nuclei (Table I). The ground-state shape of ^{61}Ga is prolate in all the four RMF parameter sets, and the quadrupole deformation parameter $\beta_2 \sim 0.22$ reproduces very well the value of the microscopic-macroscopic MMa model. The ground-state spin is $1/2^-$ according to NL1 and $3/2^-$ according to NL-SH, TM1 and NL3. The last odd proton is bound by -1, -0.9, -1.6 and -0.9 MeV, respectively. The MMa model proposes a spin of $1/2^-$ for ^{61}Ga, in agreement with the NL1 prediction. It is to be noted that sometimes there are several levels near the Fermi surface available to the odd proton. Then we blocked those levels in turn and chose the solution which corresponds to the maximum binding. However, we also noticed that two (or more, typically in spherical configurations) different blocked solutions may be very close in energy and deformation. In such cases it is difficult to select the ground-state solution. For example, this situation arises for the prolate shape of ^{61}Ga with the NL3 set. We find a binding energy of 511.27 MeV ($\beta_2 = 0.225$) when we block the $[312]3/2^-$ level, whereas the binding energy is 511.03 MeV ($\beta_2 = 0.228$) when the level $[310]1/2^-$ is blocked. In the tables we present the result which corresponds strictly to the maximum binding. In the ^{65}As nucleus the prolate and oblate solutions have very similar energies. Excepting NL1 where the prolate shape has a $3/2^-$ spin, the spin of both solutions

TABLE III. Same as Table I for ^{85}Tc, ^{89}Rh, ^{93}Ag, and ^{97}In.

	Set	ϵ_p	$[Nn_3\Lambda]\Omega^\pi$	β_2	B
^{85}Tc	NL1	−0.93	[413]5/2$^+$	−0.22	699.6
		−1.27	[431]3/2$^+$	0.09	699.3
	NL-SH	−1.24	[413]5/2$^+$	−0.22	696.9
		−0.40	[301]3/2$^-$	0.31	694.6
	TM1	−0.71	[413]5/2$^+$	−0.22	698.1
		−1.06	[431]3/2$^+$	0.09	696.0
	NL3	−0.98	[413]5/2$^+$	−0.22	695.6
		−1.35	[431]3/2$^+$	0.09	692.6
	MMa		3/2$^+$	0.05	
	MMb		[422]5/2$^+$	−0.25	
^{89}Rh	NL1	−1.30	[422]5/2$^+$	0.16	733.0
		−0.46	[411]3/2$^+$	−0.22	730.1
	NL-SH	−0.62	[411]3/2$^+$	−0.20	728.7
		−1.25	[310]1/2$^-$	0.21	726.2
	TM1	−1.04	[422]5/2$^+$	0.15	728.4
		−0.10	[411]3/2$^+$	−0.21	727.6
	NL3	−1.33	[422]5/2$^+$	0.15	726.3
		−0.40	[411]3/2$^+$	−0.21	726.2
	MMa		5/2$^+$	0.05	
	MMb		$g_{9/2}$	0.01	
^{93}Ag	NL1	−1.01	[413]7/2$^+$	0.15	766.4
		−1.38	[411]3/2$^+$	−0.08	763.7
	NL-SH	−1.47	[413]7/2$^+$	0.14	760.6
		−0.66	[411]1/2$^+$	−0.18	759.4
	TM1	−0.82	[413]7/2$^+$	0.14	760.8
		−1.14	[411]3/2$^+$	−0.08	758.5
	NL3	−1.09	[413]7/2$^+$	0.14	759.9
		−0.47	[411]1/2$^+$	−0.18	755.8
	MMa		7/2$^+$	0.05	
^{97}In	NL1	−1.01	[404]9/2$^+$	0.08	800.2
	NL-SH	−1.46	[404]9/2$^+$	0.07	796.2
	TM1	−0.84	[404]9/2$^+$	0.08	793.4
	NL3	−1.10	[404]9/2$^+$	0.08	793.8
	MMa		9/2$^+$	0.05	

is $1/2^-$. The ground state corresponds to the prolate shape, with a deformation $\beta_2 \sim 0.23$ as in the MMa model. The MMa spin is $3/2^-$, as with NL1. For the ground state of ^{69}Br the Nilsson orbital occupied by the odd proton is $[404]9/2^+$ in the four relativistic sets, which agrees with the MMa [33] and MMb [4] calculations. The RMF suggests an oblate ^{69}Br ground state with a deformation β_2 around -0.29, similarly to the MM models.

For ^{73}Rb, ^{77}Y, and ^{81}Nb (Table II) we find different solutions that often have close binding energies. In detail, for the ^{73}Rb nucleus the most bound solution is oblate ($\beta_2 \sim -0.35$) and the proposed spin is $7/2^+$ in all the parameter sets. The MM models, however, predict a prolate shape with $\beta_2 \sim 0.4$ and spin $3/2^+$ (MMa) or $3/2^-$ (MMb), which agrees better with the RMF prolate solution. For ^{77}Y we find a large prolate deformation in the ground state, with the exception of TM1 that predicts an oblate ground-state shape. Apart from the case of NL1, we also find a spherical $1/2^-$ ($p_{1/2}$) configuration that appears as an excited state, though for TM1 it coexists with the oblate ground state. In TM1 the prolate solution lies at an excitation energy of about 1 MeV. Ignoring this energy difference, then $[422]5/2^+$ is the last proton orbit of ^{77}Y in all the parameter sets which is supported by the MM predictions. Comparing the various solutions for ^{81}Nb, we find that NL1 gives a nearly spherical $9/2^+$ ground state, NL-SH and NL3 predict a highly prolate $1/2^+$ ground state (like the MM models) and TM1 gives coexistent oblate and almost spherical $9/2^+$ shapes. (Actually, configurations of spin $7/2^+$, $5/2^+$, $3/2^+$, and $1/2^+$ with nearly zero deformation are found lying at energies very close to that of the $9/2^+$ configuration and all them originate from the spherical $g_{9/2}$ shell.) If we take into account that the RMF calculation has some uncertainty, or the increase in binding after performing angular momentum projection calculations (which is particularly sizable for solutions with a large deformation [32]), and assuming the highly deformed shape as the ground state, then the Nilsson orbit of the last occupied proton is $[431]1/2^+$ in accordance with the microscopic-macroscopic calculations. The single-particle energy of the valence proton in the spherical state of ^{81}Nb with the NL1 and TM1 sets is positive. In such a case the system is unstable against proton emission and we have included these solutions only for completeness.

The RMF sets yield an oblate ground state for ^{85}Tc (Table III), with $\beta_2 = -0.22$ and a Nilsson orbit $[413]5/2^+$ for the last occupied proton. There appears a nearly spherical $3/2^+$ configuration, which for NL1 is degenerate in energy with the oblate shape. The MMa and RMF predictions do not agree, the latter being closer to the MMb solution. The ground-state shape and the Nilsson orbit are parameter dependent for the ^{89}Rh nucleus (Table III). NL1 suggests a $\beta_2 = 0.16$ solution of spin $5/2^+$, similarly to MMa, NL-SH points to a $\beta_2 = -0.20$ shape of spin $3/2^+$, and for TM1 and NL3 the prolate and oblate solutions nearly have the same energy. The MMb model favors a spherical configuration. We find low-lying prolate and oblate solutions for ^{93}Ag. The oblate solution is close to sphericity in the case of NL1 and TM1. The ground-state corresponds to a $[413]7/2^+$ orbit with a $\beta_2 \sim 0.14$ deformation. The RMF parameter sets predict nearly spherical solutions for the ^{97}In nucleus, due to approaching the $Z=50$ magic number. For both ^{93}Ag and ^{97}In, the RMF and MMa proposed ground states compare well.

Next we analyze the results for the recently observed $Z = N+1$, $T_z = -1/2$ nuclei ^{77}Y, ^{79}Zr, and ^{83}Mo. The properties of ^{77}Y have already been presented earlier and those of ^{79}Zr and ^{83}Mo are displayed in Table IV. In ^{79}Zr and ^{83}Mo the last odd nucleon is a neutron, and the spin and parity are decided by this last valence neutron. We found three solutions (prolate, spherical, and oblate) for ^{79}Zr with all the parameter sets. NL1 and TM1 predict a spherical shape of spin $1/2^-$ for the ground state, whereas NL-SH and NL3 favor a largely prolate ground state ($\beta_2 \sim 0.5$) of spin $5/2^+$.

TABLE IV. RMF results for the binding energy (B), the quadrupole deformation parameter (β_2), and the single-particle energy $\epsilon_{\rm n}$ and Nilsson orbit $[Nn_3\Lambda]\Omega^\pi$ of the state occupied by the odd neutron are shown for the nuclei ^{79}Zr and ^{83}Mo. The MMa values are from Ref. [33]. The energies are in MeV.

	Set	$\epsilon_{\rm n}$	$[Nn_3\Lambda]\Omega^\pi$	β_2	B
^{79}Zr	NL1	−15.57	$p_{1/2}$	0.00	655.0
		−14.28	$[422]5/2^+$	0.49	653.2
		−14.19	$[404]9/2^+$	−0.18	652.3
	NL-SH	−14.61	$[422]5/2^+$	0.48	652.6
		−14.79	$[404]9/2^+$	−0.18	647.2
		−14.31	$p_{1/2}$	0.00	645.7
	TM1	−14.83	$p_{1/2}$	0.00	652.9
		−14.20	$[404]9/2^+$	−0.18	651.8
		−13.85	$[422]5/2^+$	0.50	650.2
	NL3	−14.31	$[422]5/2^+$	0.49	650.3
		−14.92	$p_{1/2}$	0.00	648.5
		−14.40	$[404]9/2^+$	−0.18	647.7
	MMa		$5/2^+$	0.43	
^{83}Mo	NL1	−13.60	$[404]9/2^+$	−0.05	684.4
		−14.61	$[413]7/2^+$	−0.22	683.9
		−15.64	$[301]3/2^-$	0.27	679.1
	NL-SH	−15.11	$[413]7/2^+$	−0.21	680.4
		−14.26	$[303]5/2^-$	0.38	679.5
		−14.26	$[404]9/2^+$	−0.05	675.2
	TM1	−14.49	$[413]7/2^+$	−0.22	682.8
		−13.58	$[404]9/2^+$	−0.05	681.3
		−14.69	$[301]3/2^-$	0.27	678.4
	NL3	−14.75	$[413]7/2^+$	−0.22	679.7
		−13.79	$[404]9/2^+$	−0.05	677.6
		−14.80	$[301]3/2^-$	0.27	675.5
	MMa		$7/2^+$	−0.21	

The spin of the oblate solutions ($\beta_2=-0.18$ for the four parameter sets) is $9/2^+$. The RMF ground-state solution for the ^{83}Mo nucleus prefers an oblate shape in the NL-SH, TM1, and NL3 sets with a spin of $7/2^+$. On the other hand, NL1 suggests an oblate ($7/2^+$) and almost spherical ($9/2^+$) shape coexistence nature. Once more, the properties of the ground state are in consonance with the MMa predictions.

Among the odd-Z nuclei studied here, only ^{61}Ga, ^{65}As, ^{77}Y, and ^{89}Rh have been observed in experiment (see Janas *et al.* [4] and Refs. [6–12] quoted therein). The experimental evidence suggests that ^{69}Br, ^{73}Rb, ^{81}Nb and ^{85}Tc are proton unstable, with upper limits of 100 ns and less for their lifetimes. The stability of ^{77}Y in this region is particularly interesting and may be a consequence of the shape polarizing effect of the $N=Z=38$ core [4]. With increasing Z one would expect these odd-Z nuclei to become more spherical and the odd proton to be more bound due to the influence of the $N=Z=50$ core. However, to our knowledge, ^{93}Ag and ^{97}In have not been observed and ^{89}Rh remains the heaviest nucleus identified in this odd-Z region so far.

Calculations of the one-proton separation energy $S_{\rm p}$ are crucial for predicting the stability of isotopes near the proton drip line. The $S_{\rm p}$ value tells about the relative stability of the last occupied proton. The larger the value of $S_{\rm p}$, the more proton stable is the nucleus. The nucleus is likely to be unstable against proton emission if $S_{\rm p}<0$. We have calculated the one-proton separation energy from the ground-state binding energy of two neighboring nuclei using Eq. (1) and show the results in Table V. We find that all of the nuclei considered here have a positive $S_{\rm p}$ with the exception of ^{81}Nb. One should note that the determination of $S_{\rm p}$ arises from the difference of two large numbers, and a small change in the ground-state energy may alter the prediction. In this respect we should mention that the effects of the pairing correlations for the even-even $(N,Z-1)$ systems used in Eq. (1) to calculate $S_{\rm p}$ may be more noticeable than in the pairing scheme

TABLE V. One-proton separation energies $S_{\rm p}$ (in MeV) and charge radii $r_{\rm ch}$ (in fm) for the nuclei of Tables I–IV. The MMa values are from Ref. [33]. In the last column we indicate whether there is experimental evidence of the proton stability of the nucleus in question.

	NL1		NL-SH		TM1		NL3		MMa	
	$S_{\rm p}$	$r_{\rm ch}$	$S_{\rm p}$	$r_{\rm ch}$	$S_{\rm p}$	$r_{\rm ch}$	$S_{\rm p}$	$r_{\rm ch}$	$S_{\rm p}$	Stable
^{61}Ga	0.92	3.90	0.77	3.89	1.50	3.92	0.77	3.90	−0.09	Yes
^{65}As	2.06	4.02	1.30	4.00	1.86	4.02	1.78	4.01	0.13	Yes
^{69}Br	0.87	4.14	1.40	4.10	1.16	4.12	1.13	4.12	0.09	No
^{73}Rb	0.82	4.23	1.12	4.19	0.76	4.22	0.90	4.21	−0.31	No
^{77}Y	1.05	4.32	1.19	4.29	0.58	4.23	1.02	4.30	−0.26	Yes
^{81}Nb	−0.08	4.31	−0.28	4.39	−0.17	4.28	0.01	4.40	−1.00	No
^{85}Tc	1.05	4.37	1.29	4.34	0.77	4.36	1.05	4.35	−0.66	No
^{89}Rh	1.28	4.41	0.66	4.38	0.96	4.40	0.45	4.39	−0.50	Yes
^{93}Ag	0.95	4.44	1.26	4.42	0.69	4.44	1.00	4.43	−0.49	No
^{97}In	0.77	4.46	1.13	4.45	0.49	4.48	0.67	4.46	−0.34	No
^{79}Zr	3.27	4.28	2.11	4.32	2.41	4.25	1.96	4.33	2.36	Yes
^{83}Mo	1.20	4.34	0.19	4.31	1.78	4.33	1.63	4.33	1.26	Yes

adopted in our approximation. Also, other corrections that we have not taken into account, such as angular-momentum projection or correlations beyond mean field, like fluctuations, may easily shift the value of S_{p} by several hundred keV. Thus, in our calculation positive S_{p} values of about or less than a half MeV can be considered compatible with having a proton unstable system.

For all the parameter sets studied here, our RMF calculation successfully predicts the stable nature of the nuclei ^{61}Ga, ^{65}As, ^{77}Y, and ^{89}Rh and the unstability of ^{81}Nb against proton emission. The conclusion is less definite in some cases than in others (for example, ^{89}Rh turns out to be stable in the NL3 calculation but S_{p} is only about 0.5 MeV). The nuclei ^{69}Br, ^{73}Rb, and ^{85}Tc are found to be stable ($S_{\mathrm{p}} \sim 1$ MeV), contrary to the experimental evidence. The unobserved ^{93}Ag and ^{97}In nuclei should be rather proton stable according to the RMF calculations (maybe with some doubt in the case of the TM1 set). The relativistic calculations indicate the stability of the recently detected ^{79}Zr and ^{83}Mo isotopes, with the only exception of ^{83}Mo calculated with the NL-SH set. The microscopic-macroscopic MMa calculations [33] yield negative S_{p} values for most of the odd-Z nuclei of Table V. The MMa model predicts clearly that ^{79}Zr and ^{83}Mo are stable systems, but fails to point out the stability of ^{77}Y and ^{89}Rh. According to the MMa model ^{93}Ag and ^{97}In would be proton unstable nuclei.

In Table V we also display the charge radius r_{ch} for the ground-state solution. Taking into account the finite size of the proton, it is obtained from the rms proton radius as $r_{\mathrm{ch}} = \sqrt{r_{\mathrm{p}}^2 + 0.64}$ fm, where

$$r_{\mathrm{p}}^2 = \frac{1}{Z}\int_0^\infty 2\pi r\, dr \int_{-\infty}^{\infty} dz [r^2 + z^2] \rho_{\mathrm{p}}(r,z) \tag{2}$$

in cylindrical coordinates. For each nucleus the charge radii are almost equal with all the four parameter sets (the changes are generally less than 0.05 fm). We note that the magnitude of the rms radii changes little between the solutions of different deformation (again the changes are less than 0.05 fm, excluding ^{77}Y, ^{79}Zr, and ^{81}Nb where we have found maximum differences of ~ 0.1 fm between the various shapes). Hence we only show the charge radii of the ground-state solutions.

IV. SUMMARY AND CONCLUSIONS

In summary, we have calculated the binding energy and the quadrupole deformation parameter for odd $Z = N + 1$, $T_z = -1/2$ nuclei in the relativistic mean field model. The odd nucleon has been treated by the blocking procedure. The spin of the intrinsic states of the blocked nucleon, which is the resultant spin of the isotope, has been determined. The RMF calculations produce two or three different solutions for most of the $Z = N + 1$ nuclei in the considered valley. In some of the cases the isomeric solutions are very close to one another and can be considered as coexistent shapes.

Shapes with large deformations are predicted near the proton drip line in agreement with the microscopic-macroscopic calculations [4,33]. The spin of the $Z = N + 1$ nuclei is well reproduced in comparison with the microscopic-macroscopic model, especially if one ignores the difference in binding energy between the various shape-isomeric states. The one-proton separation energies are found to be force dependent, but the four parameter sets studied generally agree in the trends predicted for S_{p}. Overall the RMF predicts slightly bound configurations for the investigated systems. In the case of the ^{81}Nb nucleus S_{p} is negative or zero, which indicates that the isotope is just beyond the stability line. In the present calculations the nuclei ^{69}Br, ^{73}Rb, and ^{85}Tc are proton bound. Experimentally these isotopes are unstable, with estimated half-lives of less than about 100 ns [4]. The so-far unobserved nuclei ^{93}Ag and ^{97}In are found to be rather proton stable. We have checked for the NL3 parameter set that most of the nuclei studied in this work are the predicted lightest stable odd isotopes. The exceptions are arsenic and zirconium for which the lightest proton stable isotopes are ^{63}As and ^{77}Zr, respectively.

We observe that the S_{p} values, and in some cases the energy differences between oblate and prolate or spherical solutions, are of the same order as the uncertainty in the binding energies of the present RMF calculations. To further avoid ambiguities in the prediction of separation energies and ground-state shapes, a more sophisticated RMF approach for binding energy calculations would be called for. In this connection the Dirac-Hartree-Bogoliubov approach is a prescription to treat the pairing effects in a more proper way [28–30]. Finally, it should be remarked that in this work we have been concerned with bulk properties, such as binding energies, nuclear deformations, and the average properties of the intrinsic states, and not with the spectroscopy of the bands in the studied nuclei. Therefore, only the intrinsic states have been considered. To project out onto good angular momentum states remains an interesting problem for future investigations of the relativistic mean field model.

ACKNOWLEDGMENTS

The authors would like to acknowledge support from the DGICYT (Spain) under Grant No. PB98-1247 and from the DGR (Catalonia) under Grant No. 1998SGR-00011. S.K.P. thanks the Spanish Education Ministry (Grant No. SB97-OL174874) for financial support and the Departament d'Estructura i Constituents de la Matèria of the University of Barcelona for kind hospitality.

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