Unveiling the origin of shape coexistence in lead isotopes

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Abstract

The shape coexistence in the nuclei $^{182-192}$Pb is analyzed within the Hartree-Fock-Bogoliubov approach with the effective Gogny force. A good agreement with the experimental energies is found for the coexisting spherical, oblate and prolate states. Contrary to the established interpretation, it is found that the low-lying prolate and oblate $0^+$ states observed in this mass region are predominantly characterized by neutron correlations whereas the protons behave as spectators rather than playing an active role.

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The experimental information about the phenomenon of shape coexistence in atomic nuclei has been rather scarce until recent years. Nowadays this topic is one of the most active research fields in Nuclear Physics and rather widespread in the Nuclide Chart. Nowhere, however, coexistence appears as clear and impressive as in the neutron deficient lead isotopes \( (N \sim 104) \). There the ground state and the first two excited states are \( 0^+ \) states, all the three are within 1 MeV and each of them corresponds to a different shape: the ground state is spherical, one excited state is prolate and the other one oblate. The fact that this situation takes place in several lead isotopes makes this region more attractive to theoretically understand the phenomenon of coexistence. Since many years there has been considerable interest in this region and quite a few theoretical studies have tried to disentangle the main features of this coexistence. The older works were done in the frame of the Strutinsky method \( [2, 3, 4, 5] \) as well as in terms of a schematic SU(3) shell model calculation with degenerate major shells \( [6] \). Recent calculations beyond mean field \( [7, 8] \) have studied the stability of the mean field predictions. In particular, in Ref. \( [7] \) configuration mixing (shape fluctuations) calculations with the Gogny force in the frame of the Generator Coordinate Method as well as many-body calculations with a separable force have been performed. In Ref. \( [8] \), angular momentum conserving shape fluctuations were considered with the Skyrme interaction. All three calculations confirmed the persistence of the low-lying prolate and oblate configurations predicted in the mean field calculations. Unfortunately in these calculations with effective interactions, not much interest was devoted to understand the physics underlying the phenomenon of coexistence. In this Letter we adopt the opposite point of view: taking for granted that beyond mean field correlations do not destroy the simpler mean field predictions, we will perform a detailed study with the Hartree-Fock-Bogoliubov (HFB) approach and effective forces with predictive power to pin down the subtleties of the shape coexistence.

The “traditional” interpretation of the low-lying prolate and oblate minima in the closed shell lead isotopes is based in the \( 2p-2h \) proton configurations coming down in energy due to the pairing correlations and the proton-neutron (p-n) interaction, see \( [4, 6] \). This interpretation is still common sense today \( [1] \). In this Letter we will show that a different, much more natural, interpretation of these states emerges in a full selfconsistent calculation with an effective interaction. The calculations have been performed within the HFB approach using the finite range density dependent Gogny force (D1S parametrization) \( [9] \). Energies, \( E(q) \),
and wave functions (w.f.), $\varphi(q)$, with deformation $q$, have been calculated by the constrained HFB method, by constraining the expectation value of the mass quadrupole moment, i.e., $\langle \varphi(q) | z^2 - 1/2(x^2 + y^2) | \varphi(q) \rangle = q$. The calculations have been performed in an axially symmetric Harmonic Oscillator (HO) basis containing thirteen major shells, see also ref. [7].

![Diagram](image)

**FIG. 1:** Potential energies for the Pb isotopes as functions of $q$. The curves for $^{184-192}$Pb have been shifted in 1.5, 2.5, 3.5, 4.5 and 5.5 MeV respectively.

In Fig. 1 the HFB energy as functions of $q$ is displayed for the isotopes $^{182-192}$Pb. All these nuclei have spherical ground states, giving us a clear indication of the very strong signature of the $Z=82$ proton shell closure. Additional low-lying minima around 10b on the prolate and around $-7b$ on the oblate side appear indicating a pronounced shape coexistence. The first (second) excited states in $^{182-184}$Pb are of prolate (oblate) shape with deformation parameters $\beta_2 = 0.29, 0.32$ and $0.29 (-0.18, -0.18$ and $-0.20$) respectively. For $^{188-190-192}$Pb, the relative positions of the deformed minima are exchanged. The first (second) excited states of oblate (prolate) shape with $\beta_2 = -0.20, -0.20$ and $-0.17 (0.28, 0.25$ and $0.22$) respectively. It is interesting to notice that the oblate minima become more pronounced with increasing neutron number while the prolate ones display the oppo-
site trend, in particular, the prolate minimum in $^{192}\text{Pb}$ is rather shallow. On the other hand, the changes taking place on the prolate side of the potential are stronger than on the oblate one. The excitation energies of the lowest-lying oblate and prolate minima in $^{182-192}\text{Pb}$ are compared in Fig. 2 with the available experimental data [1, 10, 11, 12, 13, 14, 15, 16, 17, 18]. The crossing of the theoretical prolate and oblate states takes place at $A = 188$, two units higher than suggested by the experiment ($A=186$) [10]. It is interesting to notice that the agreement with the experiment is better for the first excited states than for the second ones independently of their oblate or prolate shape. A similar tendency has been obtained in [8].

The results obtained for the excitation energies, without further adjustment of the force, indicate that though the mean field approximation does not reproduce quantitatively the experimental results it provides a good qualitative description of the three minima. We will now try to understand the physics behind them.

An interesting issue in mean field calculations are the single particle energies (s.p.e.) corresponding to the eigenvalues of the one-body Hamiltonian $h$. In Fig. 3 the s.p.e. for protons and neutrons around the Fermi level are plotted for the nucleus $^{186}\text{Pb}$ as an example. We observe that the first level crossings in the Fermi surface appear around $|3|b$ for the neutron system and for the proton system, due to the $Z = 82$ shell closure, around $|6|b$. According to the assignment of earlier works [5, 6] the prolate minimum lying around 10 b
FIG. 3: Single particle energies of the nucleus $^{186}$Pb. Dashed (full) lines correspond to negative (positive) parity states. The thick lines represent the chemical potentials.

is a proton 4p-4h state, while the oblate one around $-7$ b is a proton 2p-2h. This labeling is somewhat misleading because the reference state of the p-h excitations is changing with deformation. In the framework of Fig. 3 it is more appropriated to talk about level crossings, one level crossing for the oblate state and two for the prolate one. The neutron systems are characterized by more crossings due to the fact that the first level crossing already takes place at $|3|b$. For a genuine determination -in the spirit of the shell model- of the p-h excitations at a given $q$ one should calculate the single particle occupancies $\nu(lj, q) = \langle \varphi(q) | \sum_{n,m} a^\dagger_{nljm} a_{nljm} | \varphi(q) \rangle$ with $a^\dagger_{nljm}, a_{nljm}$ the particle creation and annihilation operators of the spherical HFB solution. For each $(lj)$ the quantity $\Delta \nu(lj) = \nu(lj, q) - \nu(lj, q = 0)$ represents the relative spherical total single particle occupancy of the orbital $lj$ at a given deformation $q$ with respect to the corresponding one at zero deformation and is plotted in Fig. 4 again for the nucleus $^{186}$Pb. The proton w.f. of the prolate (oblate) minimum corresponds to a 7p-7h (4.5p-4.5h) with respect to the spherical state. The 7p are distributed,
mainly, within the $h_{9/2}$, $f_{7/2}$ and $f_{5/2}$ orbitals while the 7h are made, mainly, in the $h_{11/2}$ orbital. The 4.5p-4.5h of the oblate minimum are distributed within the same orbitals (with the exception of the $f_{5/2}$). The neutron w.f. of the prolate (oblate) minimum corresponds to a 5.5p-5.5h (4.4p-4.4h) with respect to the spherical state. The 5.5p are distributed, mainly, within the $i_{13/2}$ and the $g_{9/2}$ orbitals while the 5.5h are made in the $h_{9/2}$, $f_{7/2}$ orbitals. The 4.4p of the oblate minimum are distributed within the $f_{5/2}, p_{3/2}$ orbitals, the hole orbitals are the same as in the prolate case. It is interesting to observe that for small $q$ values, the particle occupation numbers change much earlier than expected from Fig. 3. For both the proton and neutron systems already at $|q| \geq 3$ barn there are significant changes. This feature is related with pairing and with the fact that in Fig. 3 one can not realize the $nlj$ mixing since the lines correspond to s.p.e. of a given $K$. In the upper part of Fig. 4 the proton and neutron pairing energies are plotted. As expected the proton pairing energy is zero at and around the spherical shape but rather large for $|q| \geq 3b$. The neutron pairing energy is very large for small $|q|$ values and decreases quite fast for large $|q|$ values. We mentioned above that the oblate and the prolate minima are the two first excited states above the ground state, the reason is that the lowest two quasiparticle states build on the ground state lie much higher, for protons ($E_{p-h}^{\text{min}} = 5.7 \text{ MeV}$) due to the large s.p.e gap of the shell closure and for neutrons ($E_{2^{+}}^{\text{min}} = 3.6 \text{ MeV}$) because of the huge pairing energy. The behavior of the pairing energies for the other lead isotopes are not very different from the plotted ones.

In our study of occupancies we got different results than the ones obtained in earlier calculations 5, 6. These occupancies, however, do not tell us directly the mechanism to generate the energy minima. To unveil the origin of the different minima let us now analyze the different energy contributions. The total HFB energy can be separated as $E_T = E_{T\nu} + E_{T\pi}$ for protons and neutrons and additionally $E_{T\pi} = E_\pi + E_C$, with $E_C$ the Coulomb energy and $E_\pi$ the pure nuclear energy. These energies, relative to the spherical shape, have been plotted in Fig. 3 for the nuclei $^{184}$Os and $^{186}$Pb. We have included the $^{184}$Os ($N = 108, Z = 76$) results in order to illustrate the behavior of a system close to $^{186}$Pb but without the impact of the $Z = 82$ shell closure. Let us first discuss the $^{184}$Os case. For $E_{T\nu}$ the proximity to the mid-shell $N = 104$ favors deformed neutron minima as we can see in the 5 MeV deep prolate and oblate minima. The 6-hole proton system would prefer a spherical or a not very pronounced deformed minimum. However, due to the p-n interaction the proton system is driven to deformed minima about 2 to 3 MeV
FIG. 4: Lower panels: Relative single particle occupations of the levels around the Fermi surface for $^{186}\text{Pb}$ as a function of $q$. Top panel: Pairing energies as a function of $q$. 
FIG. 5: The relative total energy $\Delta E = E(q) - E(q = 0)$ and its different contributions as a function of $q$ for the nuclei $^{184}\text{Os}$ and $^{186}\text{Pb}$.

depth. The behavior of $E_C$ can be classically understood, it should be a maximum at the spherical shape and rather flat around this shape corresponding to the fact that for small deformation parameters $\beta$ the correction to the spherical $E_C$ is proportional to $\beta^2$. For quadrupole moments $-5b \leq q \leq 6.5b$, both $E_\pi$ and $E_C$ are decreasing functions. The coherent addition of $E_{T\nu}$ and $E_{T\pi}$ in this $q$ range gives a $E_T$ with two very well defined deformed minima. The spherical shape however remains an energy maximum. Concerning the nucleus $^{186}\text{Pb}$, the energy minimum of $E_\pi$ is, as expected, at the spherical shape because of the magic number $Z = 82$. Small deviations around this shape increase this energy in a parabolic way until the single particle occupancies change in a sizable amount, see Fig. 4. At larger $q$ values one can distinguish the additional level crossings. $E_{T\pi}$ is rather flat for
not too large deformations being larger than zero only for $-13b \leq q \leq 13b$. It displays a very shallow minimum around $q \approx 10b$ and a second one around $q \approx 16b$. On the oblate side we find a flat maximum (!) around $-7b$ and some level crossings at higher $q$ values. Concerning $E_{T\nu}$ we find a very flat maximum around the spherical shape and two minima, one on the prolate ($q \approx 10b$) and one on the oblate side ($q \approx -7b$) as well as two shoulders at larger deformations. Around the spherical maximum we find a parabolic behavior for the same reasons as in the proton case. It is interesting to observe the presence of shoulders in $E_\pi$ at the same $q$ values where the neutron system has minima or shoulders, this is due to the p-n interaction. $E_T$ displays three minima, corresponding to spherical, prolate and oblate shapes. The deformed minima appear at exactly the same quadrupole moments as for the neutron energy. That means according to this picture the protons drive the system to the spherical ground state while the neutrons are responsible for the deformed minima. The coexistence phenomenon in the neutron deficient lead isotopes can be viewed from a microscopic point of view as the result of the following features: As we have seen in the $^{184}$Os plot, in the absence of the shell closure the proton system will display a maximum at the spherical shape and two deformed minima and so will do the neutron system. In the presence of a strong proton shell closure, $E_\pi$ together with $E_C$ provide a spherical minimum and a rather shallow $E_{T\pi}$ surface at $-15b \leq q \leq 20b$. Furthermore, the p-n interaction drives the neutron system to a spherical shape providing a very flat $E_{T\nu}$ surface around zero quadrupole moment though not a minimum. This energy flattening causes that the prolate-spherical and spherical-oblate energy barriers become very small. Notice also that due to the strong shell closure $E_\pi$ grows faster that $E_C$ decreases around the spherical shape (contrary to $^{184}$Os). This effect causes in $^{186}$Pb a cancellation of $E_{T\pi}$ with $E_{T\nu}$ in the prolate and oblate minima in such a way that the deformed minima of $E_T$ lie close to the spherical minimum. From the previous discussion we can infer that the existence of spherical, prolate and oblate states within 1 MeV is a very special characteristic of this mass region favored by the mid-shell $N = 104$ neutron configuration and the proton shell closure. The p-n and the pairing interactions provide the remaining ingredients.

We shall now try to understand the evolution of the shape coexistence with the neutron number. In Fig. 6 the different energies for the nuclei $^{182-192}$Pb are plotted. The $E_C$’s are not drawn because for all isotopes they look rather similar to the one depicted in Fig. 6 for $^{186}$Pb. In Fig. 6 we can follow very clearly the evolution of the prolate and oblate minima. In the
upper part for the nuclei with a prolate first excited state, i.e., $^{182-186}_{\text{Pb}}$, we can observe how the neutron oblate well gets deeper with increasing neutron number. The prolate minimum does the same though to a lesser extend. This can be understood looking at Fig. 3 where we can see on the oblate side, around $q = -7$ b, that for neutron numbers $N = 100, 102$ and 104
we are filling down-sloping $i_{13/2}$ orbitals. On the prolate side and around $q = 10$ b, there are down- and up-sloping orbitals providing a smaller change in the energy. In the lower part of Fig. 6 we have plotted the energies for those nuclei with an oblate first excited state, i.e., $^{188-192}$Pb. With increasing neutron number we observe a small decrease of the oblate well and the disappearance of the prolate well. This behavior can be understood again looking at Fig. 3: there we find that for neutron number $N = 106, 108$ and $110$ and around $q = 10$ b we are filling different up-sloping orbitals. On the oblate side, on the other hand, we are filling on the average orbitals without a well defined behavior. Since the behavior around the spherical minimum, $-5b \leq q \leq 5b$, is dominated by the proton behavior through the p-n interaction, $E_{T\nu}$ does not change in this region. Concerning the $E_\pi$ we find that as expected they do not vary as much as the neutron ones. We can furthermore observe the effect of the p-n interaction: In the places where $E_{T\nu}$ presents stronger variations so does $E_\pi$, see the oblate side in $^{182-186}$Pb and the prolate side in $^{188-192}$Pb. $E_{T\pi}$ does not show a clear behavior on the oblate side. Around the prolate minimum and for the nuclei $^{182-186}$Pb it shows flat minima and for $^{188-192}$Pb somewhat more pronounced ones. This behavior as explained above is caused to the p-n interaction. The addition of $E_{T\pi}$ and $E_{T\nu}$ provides $E_T$ already discussed in Fig. 1.

In conclusion the shape coexistence phenomenon in the lead isotopes has been analyzed in the selfconsistent HFB approach with the Gogny force. We have found a reasonable good description of the experimental energies as well as clear explanations for the existence of the three low-lying states of different shapes and of the evolution of these minima with the mass number. In particular, we have shown that the “traditional” understanding of shape coexistence in the lead isotopes based on proton excitations has to be modified because the proton potentials display either maxima or very shallow minima at the corresponding quadrupole moments.

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[1] A.N. Andreyev, Nature 405 (2000) 430
[2] F.R. May et al., Phys. Lett. B68 (1977) 113
[3] R. Bengtsson and W. Nazarewicz, Z. Phys. A334 (1989)269
[4] K. Heyde et al., Phys. Lett. B218 (1989)287
[5] W. Nazarewicz, Phys. Lett. B305 (1993)195
[6] K. Heyde et al., Nucl. Phys. A466 (1987)189
[7] R.R. Chasman et al., Phys. Lett. B513 (2001)325
[8] T. Duguet et al., Phys. Lett. B559 (2003)201.
[9] J. F. Berger et al., Nucl. Phys. A428 (1984) 23c.
[10] R.Julin et al., J. Phys. G27 (2001) R109.
[11] J.Heese, et al. Phys. Lett. B302 (1993) 390.
[12] R.G.Allat et al. Phys. Lett. B437 (1998) 29.
[13] P.Van Duppen et al., Phys. Rev C35 (1987) 1861.
[14] P.Van Duppen et al., Phys. Lett. B154 (1985) 354.
[15] P.Dendooven et al. Phys. Lett. B226 (1989) 27.
[16] G.D.Dracoulis et al. Phys. Lett. B432 (1998) 37.
[17] J.F.C.Cocks et al., Eur. Phys. J. A3 (1998) 17.
[18] D.G.Jenkins et al., Phys. Rev C62 (2000) 021302.