# Woods-Saxon potential parametrization at large deformations for plutonium odd isotopes 

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#### Abstract

The structure of single-particle levels in the second minima of ${ }^{237,239,241} \mathrm{Pu}$ was analyzed with the help of an axially-deformed Woods-Saxon potential. The nuclear shape was parametrized in terms of the cassinian ovaloids. A parametrization of the spin-orbit part of the potential was obtained in the region corresponding to large deformations (second minimum), depending only on the nuclear surface area. With this parametrization, we were able to reproduce successfully the spin, parity and energies of the rotational band built on the $8 \mu$ s isomeric state in ${ }^{239} \mathrm{Pu}$ and, also, a spin assignment for both isomeric states in ${ }^{237} \mathrm{Pu}$ and ${ }^{241} \mathrm{Pu}$ was carried out.


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## 1 Introduction

The theoretical description of the fission process is one of the oldest and most challenging problems in nuclear physics. Although many aspects of the fission process have already been clarified, a consistent description of fission has not yet been found [1]. The difficulty resides in the fact that the fission process involves both collective aspects and single-particle effects superimposed on a macroscopic background.

Different aspects of fission-like properties, such as asymmetric mass division and fission isomers, are believed to be associated with single-particle effects in the vicinity and even beyond the fission saddle point. Therefore, a successful description of these phenomena depends strongly on accurate calculations of single-particle states for very deformed shapes near and beyond the saddle point.

Previous studies on single-particle states in the second well have made use, generally, of methods appropriate to small deformations and, then, extended to larger defor-

[^0]mations. For instance, Dudek and collaborators [2] have carried out a systematic work on the optimization of the Woods-Saxon potential parameters for deformed $A \geq 100$ nuclei, using a shape parametrization in terms of spherical harmonics (details in [2] and references therein). In these works, the properties of an average spin-orbit field, using both phenomenological and microscopic approches, were examined.

In general, such methods suffer from the following drawbacks: on one hand, the parametrization used to describe the geometrical shape of the potential and equipotential surfaces are inappropriate at larger deformations and, on the other hand, higher order deformation parameters are needed in the multipole expansions. In this work we use another and more convenient approach to calculate single-particle states for strongly deformed nuclear shapes. In this approach the nuclear shape parametrization is carried out by using a coordinate system based upon Cassini ovaloids, as proposed by Pashkevich [3,4]. This shape parametrization requires only a few parameters to describe a whole variety of realistic shapes in deformed nuclei (up to and beyond its separation into two fragments). In this sense, this parametrization may be considered better than the expansion in terms of spherical harmonics, extensively used in the literature.

If one is interested in the quantitative description of the properties of the fission isomeric states (known as the best superdeformed states [5]), it is necessary to pay special attention to the parametrization of the spin-orbit part of the deformed nuclear potential. Therefore, a good parametrization of the spin-orbit part of the potential, which is mostly responsible for the order of single-particle levels, is extremely important in the analysis of the properties of single-particle levels at deformations corresponding to the second minima of the total energy surfaces of fissioning nuclei. In this regard, Dudek and collaborators [6] carried out shell model calculations, in which the parameters of the deformed Woods-Saxon potential were adjusted in order to reproduce the shape properties of some known isomeric states. They showed that the parametrization of the spin-orbit potential, at fission isomeric minima, should be significantly different from the parametrization applied to the ground states, resulting, thus, in a deformationdependent parametrization of the strength $(\lambda)$ and radius ( $\mathrm{r}_{o-s o}$ ) parameters. The main features of this parametrization of the spin-orbit potential for fission isomeric states consist of both increasing the effective strength of spinorbit potential and reducing its radius parameters $\mathrm{r}_{o-s o}$. Similar results were also obtained by Hamamoto and Ogle. In all these works, however, the particular dependence of the spin-orbital potential parameters on deformation was restricted to the parametrization. Moreover, the spherical shape parametrization used in these works is not the most convenient, because it requires an expansion with several terms to describe a deformed shape. However, the study of the dependence of the spin-orbit term with deformation, could be performed by using the nuclear surface area $\mathrm{B}_{s}$. In this case, the results are applicable for any parametrization.

The identification of single-particle orbitals in the second minimum is of paramount importance because it would test the basic model assumptions, especially if one could demonstrate that the right levels are used to calculate the shell correction. Concerning fission isomeric states, extensive theoretical and experimental efforts have been done to study the properties of these states, but up to now the spin and/or parity of most of the fission isomers still remain unknown. Nevertheless, some measurements of spin-parity for the second minimum in ${ }^{236,238} \mathrm{U}$ and ${ }^{240} \mathrm{Pu}$ have been performed $[7,8]$. Therefore, the study of spectroscopic properties of isomeric states would be a perfect testing ground for the single-particle model at large deformations, as proposed in this work. ${ }^{239} \mathrm{Pu}$ is a particularly interesting nucleus to study because, among odd-Pu isotopes, it is the only nucleus in which a rotational band built on an isomeric state was identified [9]. ${ }^{237} \mathrm{Pu}$ and ${ }^{241} \mathrm{Pu}$ also have two isomeric states but, differently from the ${ }^{239} \mathrm{Pu}$ case, their spin and parities are not known. Actually, only the spin (parity unknown) of the energetically lower isomer ( $8 \mu \mathrm{~s}$ ) of ${ }^{239} \mathrm{Pu}$ is known [9]. The spin and parity of the energetically higher isomer ( 2.6 ns ) remain unknown. In the case of ${ }^{237} \mathrm{Pu}$, several attempts to do an assignment to these states were carried out, as reported in the literature, but this is still an open issue. Both experi-
ment and theory agree with the fact that the ground-state isomeric level (or the short lived isomer - 122 ns ) is expected to have lower spin compared to the excited isomeric level (or the long lived isomer - $1.1 \mu \mathrm{~s}$ ), which may have higher spin. For ${ }^{241} \mathrm{Pu}$, no spin and/or parity assignment has been done so far.

As far as ${ }^{237} \mathrm{Pu}$ is concerned we note that Dudek et al. [6] have calculated the g -factors of the $\mathrm{I}=1 / 2, \mathrm{~K}=1 / 2$ and $\mathrm{I}=3 / 2, \mathrm{~K}=1 / 2$ members of the $\mathrm{K}=1 / 2$ rotational band, and compared them with the experimental g -factor ( $\mathrm{g}=-$ 0.45 ) [10]. According to their results, the most likely interpretation of the single-particle structure and the $I^{\pi}$ values of fission isomers in ${ }^{237} \mathrm{Pu}$ is:
a) for the 122 ns isomer, $\mathrm{I}=3 / 2, \mathrm{~K}=1 / 2^{-}$is a member of the $\mathrm{K}=1 / 2$ rotational band; and b) for the $1.1 \mu \mathrm{~s}$, $\mathrm{I}=\mathrm{K}=11 / 2, \pi=-1$. Finally, for the energetically higher isomer ( 2.6 ns ) in ${ }^{239} \mathrm{Pu}$ the most likely interpretation would lead to $\mathrm{I}=11 / 2^{+}$or $\mathrm{I}=11 / 2^{-}$. The work of Dudek et al. seems to have contributed to clarify the situation concerning the assignment of spin and parity of ${ }^{237} \mathrm{Pu}$ and ${ }^{239} \mathrm{Pu}$ isomeric states but, as stressed by the authors, these assignments should be treated with some caution.

Due to these above mentioned facts, the goals of this work are:(1) to obtain an optimized set of parameters for the spin-orbit part of the axially deformed Woods-Saxon potential, which would be able to describe the experimental ground-state properties of Pu isotopes (spin, parity and the energy spacing of single-particle levels of the equilibrium deformation); this could be achieved by using a more convenient shape parametrization based upon the Cassini ovaloids. (2) To obtain an analytical expression for the strength parameter $\lambda$ and the radius parameter $\mathrm{r}_{o-s o}$, as a function of the nuclear surface area $\mathrm{B}_{s}$. With the help of this expression, we aim to make a parametrization of the Woods-Saxon potential corresponding to the deformation region of the second minima of some Pu isotopes. With this parametrization it would be possible reproduce the first rotational band built on the $8 \mu \mathrm{~s}$ isomeric state of ${ }^{239} \mathrm{Pu}$, as well as to do spin and parity assignment for the two isomeric states of ${ }^{237} \mathrm{Pu}$ and ${ }^{241} \mathrm{Pu}$.

It is important to note that this new parametrization for $\lambda$ and $\mathrm{r}_{o-s o}$ differs from that of Dudek et al. [6] in two aspects:(a) $\lambda$ and $\mathrm{r}_{o-\text { so }}$ are given as a function of the nuclear surface area $\mathrm{B}_{s}$, and not of the deformation parameters $\beta_{2}$ and $\beta_{4}$; and (b) we use a more convenient shape parametrization to describe a deformed nucleus, which is based on Cassini ovaloids.

## 2 Method of calculation

### 2.1 Nuclear shape parametrization

Our nuclear shape parametrization is carried out by using the BARRIER code developed by Garcia et al. [11]. According to this code, the deformed shape (up to and beyond its separation into two fragments) can be conveniently described by the Cassini ovaloids proposed by Pashkevich, as shown in detail elsewhere [3,12].

Considering only axially symmetric nuclear shapes, the Cassini ovaloids are taken as the first approximation to the nuclear shape. The deviation from the ovaloid shape is given by an expansion into a series of Legendre polynomials. Geometrically, the family of Cassini ovaloids is defined by [13]:

$$
\begin{equation*}
r^{2}(z, \epsilon)=\sqrt{\left(a^{4}+4(c z)^{2}\right)}-\left(c^{2}+z^{2}-\epsilon^{2}\right) \tag{1}
\end{equation*}
$$

In this equation, r and z are cylindrical coordinates; $\epsilon$ is a dimensionless quantity such that $\mathrm{c}=\epsilon R_{0}^{2} ; c$ stands for the square distance from the focus of the Cassini ovaloids to the origin of coordinates; and $a$ is a dimensionless parameter which completely defines the shape, taking into account volume conservation.

In the plane containing the symmetry axis it is defined a system of coordinates $(R, x)$, such that the coordinate line $R$ is constant. This is a Cassini ovaloid where $0 \leq R<$ $\infty$ and $-1 \leq x \leq 1$. The ( $R, x$ ) coordinates are related to the cylindrical ones $(r, z)$ by the following equations

$$
\begin{gather*}
R(z, r)=\sqrt[4]{\left[\left(z^{2}+r^{2}\right)^{2}-2 \epsilon R_{0}^{2} \cdot\left(z^{2}-r^{2}\right)+\epsilon^{2} R_{0}^{2}\right]}  \tag{2}\\
x(z, r)=\frac{\operatorname{sign}(z)}{\sqrt{2}}\left[1+\frac{z^{2}-r^{2}-\epsilon R_{0}^{2}}{R^{2}(z, r)}\right]^{\frac{1}{2}} \tag{3}
\end{gather*}
$$

In this system of coordinates, the basic shape of the nucleus is described by these equations, whith $R$ constant, determining thus the Cassini ovaloids. Therefore, the nuclear shape can be defined as a curve $R(x)$ that does not intersect any straight line $x=$ constant in more than one point. Then, we expand the function $R(x)$ into multipoles,

$$
\begin{equation*}
R(x)=R_{0}\left[1+\sum \beta_{m} Y_{m 0}(x)\right] \tag{4}
\end{equation*}
$$

Therefore, the set of parameters $(\epsilon, \beta)$ determines the nuclear shape.. The details of this parametrization are given in [3,13]. As an example, we show in Fig. $1\left(\epsilon, \alpha_{4}\right)$ as a function of $\left(\beta_{2}, \beta_{4}\right)$. As clearly seem in this figure, it is difficult to establish an analytical connection between the two set of parameters. A relation was obtained by a least-square fit of the parameters $\beta_{2}, \beta_{4}$ to the shapes described in this work by the cassinian ovaloids. By using this figure it is possible to establish a connection between the two set of parameters to describe the same nuclear shape, but for more complex shapes more coeficients are needed in the harmonic spherical expansion.

It is worth mentioning that the shortcoming associated with spherical expansion, at large deformations, refers to the inclusion of non-small terms to describe extreme nuclear shapes. In our approach, however, we can avoid this problem by using the parameter $\epsilon$, which is one of the parameters of the ovaloid basis figures, subsequently used in the expansion given by (4).

### 2.2 Nuclear potential

In order to obtain single-particle energies and wave functions, the Hamiltonian has to be diagonalized. The Hamiltonian matrix elements are calculated with the wave functions of a deformed axially symmetric oscillator potential.

The basis cut-off energy is determined in such a way that negative energy eigenvalues of the Woods-Saxon potential don't change by the addition of more harmonic oscillator shells.

### 2.2.1 The axially-deformed Woods-Saxon potential

The real potential $V(r)$ is expected to follow approximately the density distribution, as usual. One of the most used radial dependences comes from the Woods-Saxon potential, which takes into account the nuclear potential and the density distribution. This potential involves the parameters $\mathrm{V}_{0}, r_{0}$ and $a$, describing the depth of the central potential, the radius and the diffuseness parameters, respectively.

The nuclear potential is given by

$$
\begin{equation*}
V(r, z, \epsilon, \hat{\beta})=\frac{V_{o}}{1+\exp ^{\frac{d i s t(r, z, \epsilon, \hat{\beta})}{a}}}, \tag{5}
\end{equation*}
$$

where $\operatorname{dist}(\mathrm{r}, \mathrm{z}, \epsilon, \hat{\beta})$ is the distance between a point and the nuclear surface, and $\epsilon$ and $\hat{\beta}$ are deformation parameters.

The depth of the central potential is parametrized as

$$
\begin{equation*}
V=V_{0}[1 \pm \kappa(N-Z) /(N+Z)], \tag{6}
\end{equation*}
$$

with the plus sign for protons and the minus sign for neutrons. The value of the constant $\kappa$ is equal to 0.63 .

### 2.2.2 The spin-orbit potential

The spin-orbit coupling is by necessity a surface term since, in a region of constant density, the only direction with local significance is that of the particle motion and, thus, it is impossible to define a pseudovector that can be coupled to the nuclear spin. If the range of the force is small compared with the distance over which the nuclear density changes appreciably, the rapid density variation in the region of the nuclear surfaces implies that $V_{s o}$ may have a somewhat different radial dependence. However, since the main effect is still concentrated near the surface, it has be found sufficient to employ a spin-orbit potential in the simple form

$$
\begin{equation*}
V_{s o}(r, z, \epsilon, \hat{\beta})=\lambda\left(\frac{h}{2 M c}\right)^{2} \nabla V(r, z, \epsilon, \hat{\beta}) \cdot(\boldsymbol{\sigma} \times \boldsymbol{p}), \tag{7}
\end{equation*}
$$

where $\lambda$ denotes the strength of the spin-orbit potential and $M$ is the nucleon mass. The vector-operator $\boldsymbol{\sigma}$ stands for Pauli matrices and $\boldsymbol{p}$ is the linear momentum operator. This definition reduces to the familiar form at spherical shapes; it uses the most general scalar expression composed of the gradient of the potential, spin and linear momentum containing only the first power of $\boldsymbol{p}$.

### 2.2.3 The Coulomb potential

The Coulomb potential is assumed to be that corresponding to the nuclear charge $(Z-1) e$, and uniformly distributed inside the nucleus. It is computed in cylindrical coordinates by using the expression given in [3].

### 2.3 Static magnetic moments

The calculation of static magnetic moments was performed in the same way proposed in [6]. For odd-A nuclei the valence particles contribute significantly to the magnetic moment, as given by the approximate expression
$\mu_{I, K}=g_{R} I+\frac{g_{k-} g_{R}}{(I+1)}\left[K^{2}+\frac{1}{4}(2 I+1)(-1)^{I+1 / 2} b \delta_{k, 1 / 2}\right]$,
where the magnetic decoupling parameter $b$ is expressed by

$$
\begin{align*}
& b\left(g_{k}-g_{R}\right) \\
& =\left\{\left\langle K=\frac{1}{2}\right|\left[\left(g_{l}-g_{R}\right) l_{+}+\left(g_{s}-g_{R}\right) s_{+}\right]\left|\overline{K=\frac{1}{2}}\right\rangle\right\} \tag{9}
\end{align*}
$$

The single-particle structure enters into the above relations via single-particle $\left|K=\frac{1}{2}\right\rangle$ wave functions for $\mathrm{K}=\frac{1}{2}$ bands, but also via $g$-factors $\mathrm{g}_{K}$ which, for one quasiparticle excitation, are given by

$$
\begin{equation*}
g_{K}=\frac{1}{K}\langle K|\left(g_{l} l_{z}+g_{s} s_{z}\right)|K\rangle . \tag{10}
\end{equation*}
$$

The effective g -factor $\mathrm{g}_{R}$, for the rotational motion, can be analyzed from the data set for $\mathrm{K}=0$ bands of even nuclei; the resulting estimate gives $\mathrm{g}_{R} \simeq Z / A$.

The intrinsic spin g factors $g_{s}$ are calculated by

$$
g_{s}=0.7 g_{s, \text { free }}
$$

where $g_{s, \text { free }}=5.58$ and -3.82 for protons and neutrons, respectively.

### 2.4 Nuclear deformation

The first step to start the optimization of the potential parameters is to fix the appropriate value of the equilibrium deformation of the nucleus. In the shell model approach, based on mean-field potentials, this is achieved in most of the practical applications using the Strutinsky method [14]. In this work, the extremal points were calculated with the BARRIER code [11], which includes the Strutinsky method with the Pashkevich parametrization for the nuclear shape. In our calculations, the pairing energy was evaluated accordingly to the commonly used prescriptions of the BCS approach, including blocking effect [15].

The expression for the surface area $B_{s}$ in the Pashkevich parametrization is

$$
\begin{equation*}
B_{s}=\frac{1}{2} R_{0}^{-2} \int r\left[1+\left(\frac{\partial r}{\partial z}\right)^{2}\right]^{\frac{1}{2}} d z \tag{11}
\end{equation*}
$$

or,

$$
\begin{align*}
B_{s}= & \frac{1}{2 \sqrt{2}} R_{0}^{-2} c^{-2} \int_{-1}^{1} d x R\left[p-R^{2}\left(2 x^{2}-1\right)-s\right]^{\frac{1}{2}} \\
& \times\left[R^{2}+\left(1-x^{2}\right)\left(\frac{d R}{d x}\right)^{2}\right]^{\frac{1}{2}}\left(1-x^{2}\right)^{-\frac{1}{2}} p^{-\frac{1}{2}} \tag{12}
\end{align*}
$$

where $p=\left[R^{4}+2 \epsilon R_{0}^{2}\left(2 x^{2}-1\right)+\epsilon^{2} R_{0}^{4}\right]^{\frac{1}{2}}, s=\epsilon R_{0}^{2}$, and $c=\left(\frac{\frac{4}{3} R_{0}^{3}}{\int^{2} d z}\right)^{\frac{1}{3}}$.

One of our goals is to obtain a relationship between some intrinsic parameters of the Woods-Saxon potential (such as $\lambda$ and $\mathrm{r}_{o-s o}$ ) as a function of $\mathrm{B}_{s}$, which is defined as the ratio of the nuclear surface area, calculated for the experimental equilibrium deformation $\left(\beta_{2}, \beta_{4}\right)$, to the surface area of a sphere with the same volume. Therefore, it is very important to check the reliability of the deformation parameters obtained in our calculations; this is done by comparing them with available experimental results and other theoretical calculations.

The extraction of the deformation parameters from the experimental data is, in many cases, uncertain (specially for $\beta_{4}$ ) and, depending on the reaction, these values can be quite different. For instance, deformations obtained with Coulomb scattering are usually greater than those extracted from nuclear reaction data. This is probably due to the different mechanisms of these processes, but some additional errors could be attributed to the fact that the interpretation of the experimental data depends, to a certain extent, on theoretical models, and partially to differences between the geometrical parameters employed in optical model calculations.

The deformation parameters ( $\epsilon, \alpha_{4}$ ) obtained from our calculations were converted into another set of deformations $\left(\beta_{2}, \beta_{4}\right)$ and, then, compared with the experimental results of Bemis et al. [16] and with theoretical results of Gareev et al. [17]. Bemis et al. carried out precise Coulomb-excitation experiments from ${ }^{4} \mathrm{He}$ inelastic scattering in even-A nuclei, through the range of the actinides deformed region. In their work, the model-dependent deformation parameters, $\beta_{20}$ and $\beta_{40}$, were extracted from the measured E2 and E4 transition moments for a distribution of nuclear charges represented by a deformed Fermi distribution, and by a deformed homogeneous distribution.

It could be appraised in Fig. 2 the agreement between our calculations, using the proposed spin-orbit parametrization, with the sistematics obtained from the works mentioned above. Also included are calculations performed for nuclei in the vicinity of those studied in this work, in order to stress the effectiveness of this method to search for equilibrium deformations in these nuclei. So, the ( $\epsilon, \alpha_{4}$ ) parameters correspond to the ground state deformations for these nuclei. The ( $\beta_{2}, \beta_{4}$ ) parameters, corresponding to the ground state, were determined by their connection with $\left(\epsilon, \alpha_{4}\right)$ (Fig. 1). In this sense, the $\left(\epsilon, \alpha_{4}\right)$ parameters must be varied to obtain the second minimum of deformation.

## 3 Results and discussion

From one of the earliest parametrizations available in the literature [14], Dudek et al. ([6] and references therein) worked out corrections for the parameters of the deformed Woods-Saxon potential, in order to improve the agreement


Fig. 1. Parameters $\left(\epsilon, \alpha_{4}\right)$ as a function of $\left(\beta_{2}, \beta_{4}\right)$


Fig. 2. Calculated parameters $\left(\beta_{2}, \beta_{4}\right)$ as a function of the atomic mass, compared with the experimental results of Bemis et al. [16] and Gareeev et al. [17]

Table 1. Deformation parameters

|  | Deformation | Isotopes <br> 237 <br> $P u$ |  |  |
| :--- | :---: | :---: | :---: | :---: |
|  |  | ${ }^{231} \mathrm{Pu}$ |  |  |
| First | $\epsilon$ | 0.225 | 0.237 | 0.225 |
| Minimum | $\alpha_{4}$ | 0.07 | 0.065 | 0.065 |
| Second | $\epsilon$ | 0.510 | 0.505 | 0.500 |
| Minimum | $\alpha_{4}$ | 0.015 | 0.025 | -0.005 |

with experimental data on sequences of spins and parities of odd-nuclei. Earlier parametrizations were usually obtained by fitting the set of parameters to the available experimental data on spherical nuclei, specially ${ }^{208} \mathrm{~Pb}[18-$ 20].

By using the above mentioned method, deformations corresponding to the second minimum could be obtained. In Table 1 we show the deformation parameters for the ground state and the second minimum of ${ }^{237,239,241} \mathrm{Pu}$. The parameters used as starting values were taken from Chepurnov [20]. This nuclear potential reproduces satisfactorily the general features of single-particle excitations, including the experimental separation energy of pairs.

For the ground state deformation of these nuclei, small changes on $\lambda$ and $r_{0-s o}$ are introduced in order to reproduce adequately the spin-parity of the levels sequence. Using single particle states obtained by this procedure, the quasiparticle states can be calculated for the first minimum region, providing spin, parity, energy and level spacing for the ground and some low-lying states. The quasiparticle spectrum was obtained by using the semimicroscopic method [21]. In order to reproduce the level spacing at neutron resonance energies, this method uses the quantum statistical model proposed by Decowski et al [22], which takes into account shell and pairing effects calculated in the framework of the BCS model. It is used in this method a consistent form of nuclear structure description and study, wich encompasses energies as low as those of the discrete levels, and up to 10 MeV where description by means of level densities is necessary. For these higher energies, experimental data from neutron resonances are employed - see details in [21]. Therefore, we obtain a set of parameters which describes rather well the ground states. In Fig. 3 are shown the fitting results of the experimental band heads of the first minimum, for ${ }^{237,239,241} \mathrm{Pu}$, as well as of the second minimum for ${ }^{239} \mathrm{Pu}$, using the model developed in this work. An adequate spectrum description is achieved for all the cases. This is quite promissing, since it would allow the extrapolation of this methodology to the super- and hyperdeformation regions, where no experimental information is available. This set of parameters is shown in Table $2 ; \lambda$ and $\mathrm{r}_{o-\text { so }}$ for ${ }^{239} \mathrm{Pu}$ are sligthly different from those of ${ }^{237} \mathrm{Pu}$ and ${ }^{241} \mathrm{Pu}$. This is due to an anomaly in single-particle excitations of ${ }^{239} \mathrm{Pu}$. Chasman et al. [23] have shown that the trend of the level spacing, for a representative set of odd-neutron and odd-proton actinides, is quite irregular and not as smooth as could be expected from the shell model and the average nuclear potential. These anomalies in the level spacing may be due

Table 2. Parameters of the nuclear potential for the neutron system

|  |  | $V_{0}$ | $r_{0}$ | $a$ | $\lambda_{n}$ | $r_{0}^{\text {so }}$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| First | $[6]$ | 49.6 | 1.347 | 0.7 | 31.5 | 1.28 |
| Minimum | This work | 53.3 | 1.24 | 0.63 | 35.25 | 1.23 |
| Second | $[6]$ | 49.6 | 1.347 | 0.7 | 43.1 | 1.28 |
| Minimum | This work | 53.3 | 1.347 | 0.63 | 38.25 | 1.20 |

to particle-hole interactions [23,24]. It should be stressed that the goal of this work is not reproducing fine details of single-particle excitations of Pu nuclei, but only their general features.

Once an optimized set of parameters is obtained for each nucleus in the region of the first minimum, the same procedure is used in the region of the second minimum, in order to reproduce the experimental information available for the shape isomers of ${ }^{237} \mathrm{Pu}$ and ${ }^{239} \mathrm{Pu}$. In the case of ${ }^{239} \mathrm{Pu}$, the main information concerning single-particle structure of the isomers comes from the rotational band built on a ground state fission isomer [9]. For ${ }^{237} \mathrm{Pu}$ the main information comes from the measured g -factor ( $\mathrm{g}=-$ $0.45(3))$ of the short-lived fission isomer [10].

It can be observed in Fig. 4 the neutron single-particle energies obtained near the Fermi level of ${ }^{239} \mathrm{Pu}$. Also, other theoretical results available for the same isotope are shown. The standard sequence is observed in the $\mathrm{N}=148$ sub-shell, as other authors did [25-28]. However, some small variations in the order and spacing of levels near the Fermi level were observed. In this case, the experimentally accepted fact that the $145^{t h}$ neutron in $\mathrm{Pu}^{239 m 1}$ resides in the state with $\mathrm{I}=5 / 2$, was reproduced in our calculations. The possible candidates for the fission isomer state are $\frac{5}{2}^{+}|633\rangle$ and $\frac{5}{2}^{+}|622\rangle$. However, the high probability of finding $\ell$ antiparallel to the $s$ components, according to experimental results [9], limits the number of possible states. The state $\frac{5}{2}^{+}|622\rangle$ just have the opposite structure, i.e., the component with $\ell$ antiparallel to $s$, and this does not exceed $20 \%$ in our calculation. Only the state $\frac{5}{2}^{+}|633\rangle$ have the proper intrinsic structure with $\ell$ antiparallel to the $s$ components. In the case of ${ }^{237} \mathrm{Pu}$, a level $\frac{1}{2}^{-}|510\rangle$, close to the Fermi energy, appears as a likely candidate for the short-lived fission isomer (a similar result was obtained by Dudek et al [6] ). The experimental value for the g -factor $(\mathrm{g}=-0.45)$ is compatible with the rotational state ( $\mathrm{K}=1 / 2, \mathrm{I}=3 / 2$ ), with $\mathrm{g}=-0.43$.

The rotational excitations of ${ }^{239} \mathrm{Pu}$, identified by conversion electron spectroscopy [9], are compared in Fig. 3 with our calculations. The rotational bands with spin $5 / 2^{+}$, build on the 2.6 ns isomeric state in ${ }^{239} \mathrm{Pu}$, were obtained by using the "experimental" moment of inertia of the band, in accordance with the rotational constant $\mathrm{A}=3.36 \mathrm{keV}$ found in [9]. These results were partially published with the sole purpose to justify the validity of the theoretical methods used in the interpretation of ${ }^{239} \mathrm{Pu}$ electrofission and photofission data [29].



Fig. 3. The experimental band heads [30] of the first minimum, for ${ }^{237} \mathrm{Pu}$ (a), ${ }^{239} \mathrm{Pu}$ (b) and ${ }^{241} \mathrm{Pu}(\mathrm{c})$; compared with our theoretical results. In right-botton (d), the experimental spectroscopical available information of the second minimum of ${ }^{239} \mathrm{Pu}[9]$ is compared with our theoretical calculations

Fig. 4. Neutron single particle level energies of ${ }^{239} \mathrm{Pu}$ obtained in this work, compared with other results

With the set of $\lambda$ and $\mathrm{r}_{o-s o}$, for both deformation regions (first and second minima), it was possible to obtain the dependence of these parameters with the surface area term $B_{s}$. Since the main effect of the spin orbit coupling is concentrated near the surface, we have tried to obtain a parametrization for this part of the potential depending directly on the surface area term $B_{s}$, instead of as a function of the deformation parameters as proposed by Dudek et al. [6].

In Figs. 5 and 6 we present results for $\lambda$ and $\mathrm{r}_{o-s o}$ as a function of the surface parameter $B_{s}$. It is important to note that our results were normalized to the standard values given by Chepurnov [20]. The parametrization of Dudek et al. [6] is also shown in these figures. It is clear that our parametrization differs from that proposed by Dudek et al., particularly in the second minimum region. As an aproximation, we propose an exponential dependence of these parameters with the nuclear surface (see Fig. 5 and Fig. 6).


Fig. 5. Parameter $\lambda$ as a function of the surface parameter $\left(B_{s}-1\right)$. Full line: fitting; dashed line: parametrization of Dudek et al. [6]

Fig. 6. Parameter $\mathrm{r}_{o-s o}$ as a function of the surface parameter $\left(B_{s}-1\right)$. Full line: fitting; dashed line: parametrization of Dudek et al. [6]

At the second minimum region, there are several experimental works dealing with the fission isomeric state of ${ }^{239} \mathrm{Pu}$, while no experimental information is available for ${ }^{241} \mathrm{Pu}$. Nevertheless, by using the procedures adopted in this work, we obtained optimized single particle levels for ${ }^{241} \mathrm{Pu}$ (Fig. 7). A closer inspection of Fig. 7 reveals a bunch of states between -8.0 and -7.0 MeV . A large gap be-
fore two relatively close states $(5 / 2,-3 / 2)$ shows up. These two levels are the best candidates for the ${ }^{241} \mathrm{Pu}$ isomeric state. A huge gap is observed between these levels and the next pair $(5 / 2,7 / 2)$, which indicates that certainly the $(5 / 2)$ and ( $-3 / 2$ ) states might well be related with the isomeric states of this isotope. The parameters $\lambda$ and $\mathrm{r}_{0-\text { so }}$ we obtained agree with the systematics (Figs. 5 and 6).


Fig. 7. ${ }^{241} \mathrm{Pu}$ single particle levels obtained at the second minimum region

## 4 Conclusions

We have obtained a new parametrization for the spinorbit interaction using the Woods-Saxon single particle model. This study was carried out by using the Cassinian ovaloids for the nuclear shape parametrization, which is better than the parametrizations based on the spherical harmonic expansion. Also, we have obtained an exponential dependence between the parameters characterizing the spin-orbit interaction and the nuclear surface area. In this case, the strength of the spin-orbit potential increases with an increasing nuclear surface area.

With our parametrization, the single-particle structure of ${ }^{241} \mathrm{Pu}$ was calculated. There are two levels, $5 / 2^{+}$ and $3 / 2^{-}$, which are the best candidates to explain the fission isomerism in this nucleus. It is important to note that this parametrization differs from others found in the literature [6,28], particularly because, in our case, the parameters are expressed as a function of the nuclear surface area. Nevertheless, there are common characteristics as e.g. the increase of the strength of the spin-orbit potential.

Moreover, we have proposed a procedure to study the second minimum region, based not only in the study of the results of the Woods-Saxon single particle model, but based also in the study of the quasiparticle spectrum obtained with a BCS model. It is important to note that the microscopic treatment of the spin-orbit interaction is not so far well developed. Besides, the spin-orbit splitting depends on the nucleon-nucleon interaction used in microscopic calculations. So, it is not possible to compare our results with microscopic studies for this kind of effect.

Finally, we would like to point out that our approach, for the use of the Semi-Microscopic Combined Method, was succesfully employed in the calculation of the transition nucleus levels at saddle points [29], which allowed the identification, for the first time, of a concentration of M1
strength in the electro- and photofission of ${ }^{239} \mathrm{Pu}$ near the fission barrier (details in [30]).

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## References

1. J. Moreau and K, Heyde, "The Nuclear Fission Process", Ed. C. Wagemans, 277 (1991)
2. J. Dudek, Z. Szymànski, T. Werner, A. Faessler, C. Lima, Phys. Rev. C26, 1712 (1981)
3. V.V. Pashkevich, Nucl. Phys. A169, 275 (1971)
4. J. Damgaard, H.C. Pauli, V.V. Pashkevich, V.M. Strutinsky, Nucl. Phys. A135, 432 (1969)
5. D. Habs, Nucl. Phys. A502, 105 (1989)
6. J. Dudek, W. Nazarewicz, A. Faessler, Nucl. Phys. A412, 61 (1984)
7. P. Reiter, "Anregung und Zerfall des superdeformierten ${ }^{238}$ U", PhD Thesis, Univ. Heidelberg, (1993)
8. D. Pansegrau, " $\gamma$-Specktroskopie im II Minimum von ${ }^{240} \mathrm{Pu}{ }^{\prime}$, PhD Thesis, Univ. Heidelberg, (1994)
9. H. Backe, L. Richter, D. Habs, V. Metag, J. Pedersen, P. Singer, H.J. Specht, Phys. Rev. Lett. 42, 490 (1979)
10. M.H. Rafailovich, E. Dafni, G. Schatz, S.Y. Zhu, K. Dybdal, S. Vajda, C. Alonso, G.D. Sprouse, Phys. Rev. Lett. 48, 982 (1982)
11. F. Garcia, O. Rodriguez, J. Mesa, J.D.T. Arruda-Neto, V.P. Likhachev, E. Garrote, R. Capote and F. Guzman. Comp. Phys. Comm., 120, 57 (1999)
12. F.A. Ivanyuk, H. Hofmann, V.V. Pashkevich, S. Yamaji, Phys. Rev. C55, 1730 (1997)
13. R. W. Hasse, W.D. Myers, "Geometrical Relationship of Macroscopic Nuclear Physics", Spring Verlag, 83 (1988)
14. V.M. Strutinsky, Nucl. Phys. A95, 420 (1967)
15. M. Brack, J. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinsky and C. Y. Wong, Rev. Mod. Phys. 44, 320 (1972)
16. C.E. Bemis, F.R. McGovan, J.L. Ford, et al. Phys. Rev. C8, 1466 (1973)
17. F.A. Gareev, S.P. Ivanova, V.V. Pashkevich, Sov. J. Nucl. Phys. 11, 667 (1970)
18. E. Rost, Phys. Lett. B26, 184 (1968)
19. J. Blomqvist, and S. Wahlborn, Ark. Fys. 16, 543 (1960)
20. V.A. Chepurnov, Sov. J. Nucl. Phys. 6, 696 (1968)
21. F. Garcia, O. Rodriguez, V.A. Rubchenya, E. Garrote, Comp. Phys. Commun. 86, 129 (1995)
22. P. Decowski et al., Nucl. Phys. 110, 129 (1968)
23. R.R. Chasman, I. Ahmad, A.M. Friedman, J.R. Erskine, Rev. Mod. Phys. 49, 833 (1977)
24. F.A. Gareev, S.P. Ivanova, L.A. Malov, and V.G. Soloviev, Nucl. Phys. A171, 134 (1971)
25. M. C. Pauli and T. Ledergerber, Nucl. Phys. A175, 545 (1971)
26. V. Mosel and H. W. Schmitt, Nucl. Phys. A165, 73 (1971)
27. P. Moller and J. R. Nix, Nucl. Phys. A229, 269 (1974)
28. I. Hamamoto and W. Ogle, Nucl. Phys. A240, 54 (1975)
29. J.D.T. Arruda-Neto, M.-L. Yoneama, J.F. Dias, F. Garcia, M.A.V. Reigota, V.P. Likhachev, F. Guzmán, O. Rodriguez and J. Mesa, Phys. Rev. C55, 2471 (1997)
30. Richard B. Firestone, Table of Isotopes, Eighth Edition, John Wiley and Sons, New York (1996)

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