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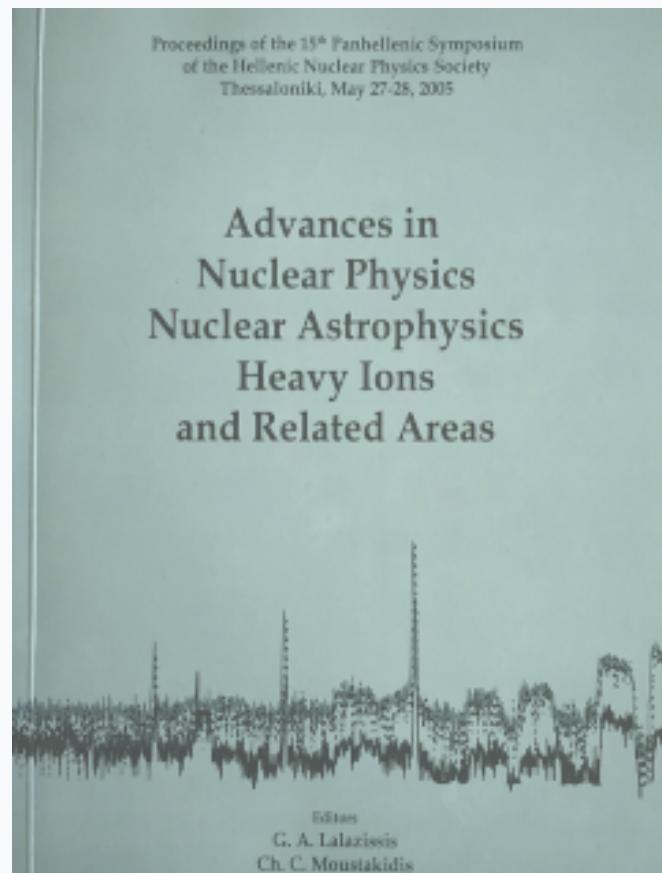
Superdeformation in Pb isotopes with large neutron excess

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Abstract

Covariant Density Functional theory (CDFT) is used to investigate superdeformation in Pb isotopes on the neutron rich side of the periodic table. Energy surfaces and deformation parameters in this region are calculated by solving the constrained Relativistic Hartree Bogoliubov (RHB) equations. We use the parameter set DD-ME2, which has an explicit density dependence as well in the isoscalar as in the isovector channel together with the finite range pairing force D1S of Gogny. With increasing neutron number we find a characteristic pattern for superdeformed minima in these nuclei.

1   Introduction

Density functional theory provides a successful and relatively simple tool to investigate the deformation landscape of heavy nuclei. This is important for the description of collective processes such as low lying vibrations or nuclear fission and fusion reactions. In recent years it has been applied in the description of superdeformed rotational bands, the investigation of shape coexistence in heavy nuclei and the calculation of fission barriers in actinides. Most of these investigations have been focused in regions of the periodic system, which are experimentally easily accessible, in particular the proton rich side. There, it is relatively easy to produce such nuclei by heavy-ion fusion reactions.

Unfortunately, this is not the case in the investigation of very heavy nuclei on the neutron rich side, since it is very difficult to produce and to investigate them experimentally. On the other hand, these nuclei are extremely important for our understanding of the nuclear synthesis of heavy elements above the Pb region. Nuclei with very large neutron excess play a dominant role on the r-process path. It is therefore of great interest to study the behavior of such

nuclei by theoretical investigations. Since there is little experimental aspect, it is important the use of the most modern theoretical tools.

In this manuscript we perform such an investigation in the framework of covariant density functional theory [1]. It is applied to the calculation of energy surfaces as a function of the quadrupole deformation of the chain of Pb isotopes, particularly those characterized by very large neutron excess. We use constraint RHB theory based on the parameter set DD-ME2 and on the Gogny interaction D1S in the pairing channel. It has been shown by Ring et al. ([2]) that this functional is particularly successful in the description of masses in heavy and superheavy nuclei as well as in the calculation of the Q_α-values in α-decay chains of recently measured super-heavy elements.

In section 2 we discuss the basis theoretical ingredients for Covariant Density Functional Theory and in section 3 we apply this method in the investigation of the behavior of neutron rich Pb isotopes as a function of the quadrupole deformation.

2   Covariant Density Functional Theory

The starting point of Covariant Density Functional Theory (CDFT) is a standard Lagrangian density [3]

$$
\begin{aligned}
\mathcal{L} = {} & \bar{\psi}\left(\gamma(i\partial - g_\omega\omega - g_\rho\vec{\rho}\vec{\tau} - eA) - m - g_\sigma\sigma\right)\psi \\
& + \frac{1}{2}(\partial\sigma)^2 - \frac{1}{2}m_\sigma^2\sigma^2 - \frac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^2 \\
& - \frac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \frac{1}{2}m_\rho^2\vec{\rho}^2 - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}
\end{aligned}
\tag{1}
$$

which contains nucleons described by the Dirac spinors ψ with mass m and three effective fields referred to the mesons σ, ρ and ω. This Lagrangian contains as parameters the meson masses m_σ, m_ω, and m_ρ and the coupling constants g_σ, g_ω, and g_ρ, as well as the two parameters g_2, and g_3 which comes from the introduction of the non-linear meson coupling. [4].Therefore, the extended form of the σ potential

$$
U(\sigma) = \frac{1}{2}m_\sigma^2\sigma^2 + \frac{1}{3}g_2\sigma^3 + \frac{1}{4}g_3\sigma^4.
\tag{2}
$$

produce the additional density dependence. By fitting to experimental data in carefully chosen spherical nuclei, over the years, several very successful parameter sets have been introduced as for instance NL1 or NL3 [3], which describe many ground state properties of finite nuclei all over the periodic table.

The density dependence in these models, however, only influences the isoscalar channel σ. The vector fields, in particular the isovector channel described by the ρ-meson, are still coupled linearly and this leads to relatively large neutron radii and a very stiff equation of state for neutron matter as well as very stiff symmetry energies as a function of the density [6]. The most modern covariant density functionals therefore eliminate the non-linear coupling terms and use instead of that coupling constants $g_\sigma(\rho)$, $g_\omega(\rho)$, and $g_\rho(\rho)$ which depend on the baryon density ρ. This concept is evidently closer to the idea of a density functional theory. In this case the energy functional derived from the energy momentum tensor of the Lagrangian (1) has the form

$$
E_{RMF}[\hat{\rho}, \phi_m] = \mathrm{Tr}\left[(\boldsymbol{\alpha p} + \beta m)\hat{\rho}\right] \pm \int \left[\frac{1}{2}(\nabla\phi_m)^2 + U(\phi_m)\right] d^3r
$$
$$
+ \mathrm{Tr}\left[(\Gamma_m(\rho)\phi_m)\hat{\rho}\right]. \tag{3}
$$

where the $+$ sign holds for scalar mesons and the $-$ sign for vector mesons. The index m is a generic notation for the various meson fields $\phi_m = \sigma, \omega_\mu, \rho_\mu$ and the electromagnetic field A_μ. The vertices read

$$
\Gamma_\sigma(\rho) = g_\sigma(\rho), \quad \Gamma_\omega^\mu = g_\omega(\rho)\gamma^\mu, \quad \vec{\Gamma}_\rho^\mu = g_\rho(\rho)\vec{\tau}\gamma^\mu, \quad \Gamma_e^\mu = e\frac{1-\tau_3}{2}\gamma^\mu, \quad (4)
$$

Of course, the choice of the density dependence in these coupling constants is essential. We use here the Typel and Wolter ansatz which has been introduced in Ref. [7], using relativistic Brückner calculations as a guideline.

Essential is also the role of pairing correlations in the description of finite nuclei with open shells. They are not contained in an energy density of the Kohn-Sham type. However they can be easy incorporated using an extended functional by replacing the normal density matrix $\hat{\rho}$, with the generalized density matrix of Valatin [8]

$$
\hat{\mathcal{R}} = \begin{pmatrix} \hat{\rho} & \hat{\kappa} \\ -\hat{\kappa}^* & 1 - \hat{\rho}^* \end{pmatrix}. \tag{5}
$$

which contains besides the normal density $\hat{\rho}$ the pairing tensor $\hat{\kappa}$.

Therefore, the RMF-functional (3) is not the final expression of the energy functional, but additional parts must be used. The one, the pairing term, has the form:

$$
E_{pair}[\hat{\kappa}] = \frac{1}{4}\mathrm{Tr}\left[\hat{\kappa}^*\hat{V}^{pp}\hat{\kappa}\right] \tag{6}
$$

with $\hat{V}^{pp}$ being a two-body pairing interaction of a Gogny form, where the succesful set D1S [9] is used. The other part comes from applying an external field, since we are interesting in calculating the energy surfaces with respect

to quadrupole deformation β_2. This constraining energy has the form:

$$E_{constr}[\hat{\rho}] = \frac{c}{2}(\text{Tr}\left[\hat{Q}\hat{\rho}\right] - q)^2 \tag{7}$$

Here, $\hat{Q}$ is the quadrupole operator, q is the actual value of the quadrupole moment and c is a stiffness parameter. Finally the full density functional, depending on $\hat{\mathcal{R}}$, i.e. on $\hat{\rho}$ and on $\hat{\kappa}$, is of the form:

$$E_{RHB}[\hat{\rho}, \hat{\kappa}, \phi_m] = E_{RMF}[\hat{\rho}, \phi_m] + E_{pair}[\hat{\kappa}] + E_{constr}[\hat{\rho}] , \tag{8}$$

3   Constraint RHB calculations for neutron rich Pb isotopes

For our calculations we have adopted the parameter set DD-ME2 [2]. This set has recently been adjusted to reproduce the properties of symmetric and asymmetric nuclear matter, binding energies, charge radii and neutron radii of 12 spherical nuclei. The parameters are given in the table below.

	DD-ME2		
m_σ =	550.1238	$g_\sigma(\rho_{\text{sat}})$ =	10.5396
m_ω =	783.000	$g_\omega(\rho_{\text{sat}})$ =	13.0189
m_ρ =	763.000	$g_\rho(\rho_{\text{sat}})$ =	3.6836

Table 1
The parameter set DD-ME2. Masses are given in MeV and the remaining parameters are dimensionless. The nucleon mass is M=939 MeV and the saturation density is $\rho_{\text{sat}} = 0.152$ fm^{-3} (from Ref. [2]).

When compared with the results obtained with DD-ME1 it is found that this interaction considerably improves the agreement with experimental data. In particular, one has obtained very good results for the masses of approximately 200 nuclei, for the isoscalar monopole and isovector dipole resonances, and excellent agreement with the recently reported α-decay chains of the new element $Z = 115$ [2].

In the present work we have performed constrained RHB calculation in the isotopic chain of Pb nuclei. Starting from the doubly magic ^{208}Pb up to very exotic isotopes with extremely large neutron excess: the heaviest ^{274}Pb nucleus, considered in the present work, has isospin ratio $N/Z = 2.37$.

The potential energy surfaces (PES) of several Pb nuclei are shown in Figures 1. The selected Pb isotopes differ from each other by six neutrons or three

units of isospin. We have not subtracted any corrections of spurious rotational contributions. It is expected that such corrections would have some influence to the energy of the stationary points in the energy surface.
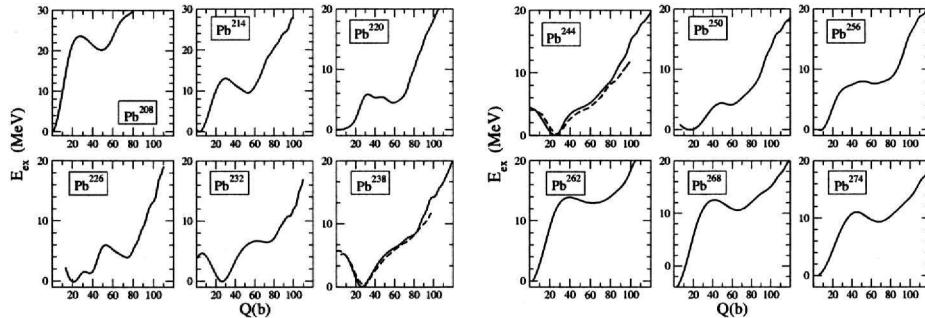

Fig. 1. *Potential energy surfaces for Pb isotopes between* ^{208}Pb *and* ^{274}Pb *as a function of the quadrupole moment Q. For* ^{238}Pb *and* ^{244}Pb *we also show for comparison calculations with the parameter set NL3 (dashed line).*

Instead of plotting absolute values of the energy, we show, in the above figures, the excitation energy E_{ex} with respect to quadrupole moment. The excitation energy is defined here as the difference between the energy of the system constraint to a certain deformation and energy $E_{g.s.}$ of the ground state minimum $E_{ex} = E_{con} - E_{g.s.}$, since this is what we are really interesting in.

The model predicts superdeformed minima at a large deformation of about $\beta_2 \sim 0.6$. However, it is seen from Figs. 1 that ^{238}Pb and ^{244}Pb practically do not show any superdeformed minimum. This fact is not a peculiarity of the present parametrization, since it also appears with the use of the successful parameter set NL3 [3]. The results of the calculations for ^{238}Pb and ^{244}Pb nuclei, are shown by dashed lines in Figures 1 where the similar behaviour can be easily seen.

In Fig. 2 several quantities of intetrest, such as the excitation energy E_{ex} of the superdeformed minimum, the quadrupole deformation parameter β_2 and the pairing energy are shown as functions of the mass number A.

4 Summary

In the present work, constrained Relativistic Hartree Bogoliubov (RHB) calculations have been used for energy surfaces and deformation parameters of very neutron rich Pb nuclei. The Lagrangian parametrization DD-ME2, which has an explicit density dependence in both isoscalar and isovector channels has been employed, while for the pairing interaction the finite range pairing force D1S of Gogny was used. This study showed the existence of superdeformed
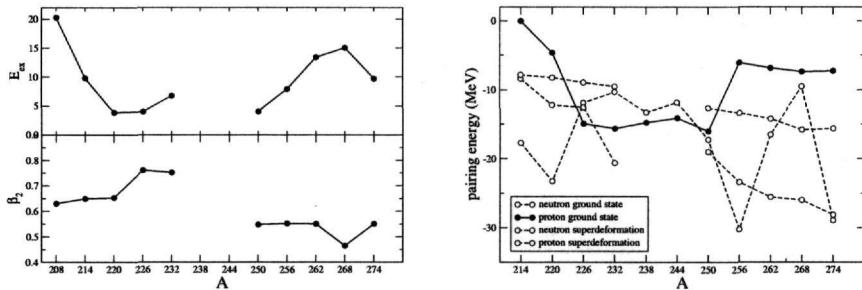
Fig. 2. *(a) Excitation energy E_{ex} and quadrupole deformation β_2 of the superdeformed minimum as a function of the mass number A of Pb nuclei.(b) Proton, neutron pairing energy with respect to A at the ground state and superdeformation.*

minima in most of Pb nuclei at excitation energies which vary from a few MeV to large values. The heights of the barrier at superdeformation are larger for those Pb isotopes which favor spherical shape. The study also showed that the results are independent of the variation of the RHB model used in the analysis.

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