Fission properties of the Barcelona-Catania-Paris energy density functional

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Abstract. Fission properties of the Barcelona-Catania-Paris (BCP) energy density functional are explored by performing constrained mean field Hartree-Fock-Bogoliubov (HFB) calculations along the fission path. These calculations provide us with the quantities required to estimate the spontaneous fission half lives and fragment mass distribution. The results obtained are compared to experimental data and other calculations.

1. Introduction
The Barcelona-Catania-Paris (BCP) energy density functional (EDF) has been proposed [1] as an alternative to more traditional approaches based on Gogny or Skyrme type functionals (see Ref [2] for a review) in the calculation of nuclear properties all over the Nuclide Chart. The definition of the BCP EDF conceptually differs from the underlying philosophy of the Skyrme or Gogny EDF’s in its use of realistic nuclear matter equations of state to inspire a finite nuclei functional by means of the Local Density Approximation (LDA). The suitability of the BCP EDF to describe finite nuclei was tested first in [1] where masses and radii of spherical nuclei were used to define the parameters of the functional (called BCP1 and BCP2). Next, the ability of BCP1 and BCP2 to reproduce quadrupole deformation properties was considered in [3]. Next in the multipole parametrization of the nuclear shape is the octupole degree of freedom, responsible of the breaking of parity symmetry in several rare earth and actinide isotopes. In [4] we studied the suitability of BCP1 and BCP2 to describe octupole deformation properties in the context of the collective Schrödinger equation (CSE). We concluded that BCP was good in reproducing experimental quantities related to octupole deformation. The results of [4] not only indicated...
the validity of the potential energy curves (PEC) but also the suitability of the collective inertias required in the CSE. Both in [3] and [4] the fission barrier of $^{240}$Pu was considered as an example of a mixed case where both quadrupole and octupole deformation play a role. The conclusion reached in both cases was that the BCP1 and BCP2 fission barriers were both rather close to the one of the Gogny D1S.

Given the relevant role of fission in establishing the very limits of existence of heavy nuclei, including the famous ”island of stability” [5] it is timely to address in a more systematic way the description of fission with the BCP functional. Fission involves a delicate balance between a variety of very different kinds of shapes that makes it a perfect testing ground to complement previous studies of deformation properties with BCP.

In this paper we present the results of fission calculations in three characteristic nuclei, two actinides ($^{246}$Cm and $^{252}$No) and a superheavy ($^{270}$Sg). Fission barrier heights and spontaneous fission half lives are given. The role played by the collective mass in the description of half lives is discussed. The differences with the results obtained with the Gogny force [6] (D1S parametrization [7]) are also discussed.

2. Methodology

The BCP energy density functional is made of a bulk part which is inspired by fully microscopic and realistic calculations of symmetric and neutron matter equations of state [8]. The two equations of state (symmetric and neutron matter) given as a function of the nuclear density are parametrized using a fitting procedure in terms of polynomials of the densities. To account for finite size effects related to the surface energy, a phenomenological finite range interaction of gaussian type is included. In addition, the Coulomb interaction and the spin-orbit term are taken exactly as in the Skyrme or Gogny forces. To deal with open-shell nuclei we include in the BCP functionals a zero range density-dependent pairing interaction fitted to reproduce the nuclear matter gaps obtained with the Gogny force [9]. The only free parameters of these functionals are the isospin like $V_L$ and unlike $V_U$ strengths of the surface term, the range of the Gaussian form factor of the surface term $r_0$ and the strength of the spin-orbit interaction $W_0$ [1]. These free parameters are adjusted in the usual way to reproduce the ground state energy and charge radii of some selected spherical nuclei. With these ingredients, the BCP functionals give an excellent description of 161 even-even spherical nuclei with rms values for the ground-state energies and charge radii comparable with the most performing of Skyrme, Gogny and Relativistic mean field type. Apart from the advantages already mentioned in [1], the BCP functionals are advantageous in their application to finite nuclei as a consequence of a reduced computational cost as compared to Gogny or even Skyrme. Recently, open questions about BCP and ways to improve the EDF have been discussed in [10].

To describe the path to fission we use mean field configurations given in terms of HFB wave functions that define the standard and pairing densities required by the BCP functional. The amplitudes of the Bogoliubov transformation defining those HFB wave functions are computed as the solution of the HFB equation. In our calculations we have recast the HFB equation in terms of the minimization of the energy. The minimization process uses the gradient method as described in [11, 12]. The most evident advantage of this method is its handling of constraints, which allows a larger number of them to be treated at once. For the calculation of fission barriers and to reduce the computational effort we have restricted the calculation to axial symmetry preserving configurations (but reflection symmetry breaking is allowed). The quasiparticle operators are expanded in an axially symmetric harmonic oscillator basis.

Dynamical parameters like quadrupole collective masses and moments of inertia are computed by recurning to the usual approximations of neglecting the interaction in the stability matrix (cranking approximation [13]).

The spontaneous fission half life is computed with the standard WKB formalism where $T_{sf}$
is given (in seconds) by

\[ T_{sf} = 2.86 \times 10^{-21} (1 + \exp(2S)). \]

The action along the \( Q_2 \) constrained path is

\[ S = \int_a^b dQ_2 \sqrt{2B(Q_2)(V(Q_2) - E_0)}. \]

For the collective quadrupole inertia \( B(Q_2) \) we have used the Adiabatic Time Dependent HFB (ATDHFB) expression computed in the “cranking” approximation [13]. The quantity \( V(Q_2) \) entering the action is the HFB energy minus the zero point energy (ZPE) correction \( \epsilon_0(Q_2) \) associated with the quadrupole motion and minus the rotational energy correction given by the rotational approximation with the Yoccoz moment of inertia (see [14, 15] for further details). Finally, an additional parameter \( E_0 \) is introduced in the action. It is meant to represent the quantal ground state energy obtained after considering quantal fluctuations in the quadrupole degree of freedom. This quantity is often taken as a free parameter or kept fixed to some reasonable value. We have followed the latter approach with \( E_0 = 0.5 \text{ MeV} \).

3. Results

Fission barrier calculations for three heavy nuclei, namely \(^{246}\text{Cm} (Z=96), ^{252}\text{No} (Z=102), \) and \(^{270}\text{Sg} (Z=106)\) are discussed. We have compared the results of the calculations with the BCP1 interaction with those obtained by using the Gogny force with the standard D1S parametrization. The reason for this comparison is the success of the Gogny D1S in describing a variety of fission related phenomena [14, 15, 16, 17, 18, 19, 20]. The BCP2 parametrization has not been considered as it gives results which are very close to the BCP1 ones. As mentioned in the previous section, axial symmetry is preserved in the calculations and therefore the first fission barrier won’t be reduced as a consequence of triaxiality. This implies that our results for the spontaneous fission (SF) half life are overestimated.

3.1. Curium

In Fig 1 several properties relevant to fission are depicted for the \(^{246}\text{Cm}\) nucleus and the two EDF considered. On the left panel the HFB energy is given as a function of axial quadrupole moment \( Q_2 \). Two fission barriers are observed in both cases. Both the inner and outer barriers are lower for BCP1 than for D1S. Please remember that the inner barrier height is very sensitive to triaxial effects not considered in this paper. The excitation energy of the fission isomer is a couple of MeV lower for BCP than for D1S. The lower energies obtained with BCP could be a consequence of the lower surface energy for BCP as compared to D1S [3]. On the right panels and from bottom to top we have the particle-particle correlation energies \( E_{pp} = \text{Tr}\Delta\kappa \) for protons and neutrons. They are systematically lower for BCP than for D1S indicating weaker pairing correlations in BCP. In the middle panel the octupole \( Q_3 \) and hexadecapole \( Q_4 \) moments are depicted. They are very similar in both calculations indicating that the shapes along the fission path are also very similar. Octupole deformation starts to develop at \( Q_2 = 50b \) (at the fission isomer position) and grows as the nucleus evolves to scission. Finally, in the upper panel the inertia \( B(Q_2) \) entering the action in the WKB formula is depicted. The BCP inertia is systematically higher than the D1S one, probably as a consequence of the weaker pairing correlations in BCP (the inertia is roughly proportional to the inverse of the pairing gap).

With some of these quantities (and others not depicted, like the rotational and zero point energy corrections) we can compute the spontaneous fission (SF) half life for this isotope. We obtain the values \( 4.310^{21} \text{ s} \) for D1S and \( 6.210^{17} \text{ s} \) for BCP1. The shorter half life given by BCP1, as compared to D1S, is the consequence of the balance between the barrier heights which are lower in BCP and favor shorter half lives and the collective inertia that is higher in BCP1.
what favors longer half lives. Both results should be compared with the experimental value $1.8 \times 10^7$ yr ($5.7 \times 10^{14}$ s) [21]. Two comments are in order, first the reduction of the first barrier due to triaxiality can lower the half lives although its impact can be softened by the increase of the collective inertias due to triaxiality [16]. The second comment has to do with the sensitivity of half lives to the $E_0$ parameter, by changing it to 1.0 MeV we obtain a half life of $1.5 \times 10^{13}$ s with BCP, meaning a reduction of four orders of magnitude in the half life.

Finally, by looking at the density matter distribution for very elongated shapes we can identify the nascent fragments and compute their mass contents. The results correspond to an asymmetric mass distribution ($Q_3$ is different from zero at large deformations) with fragments $^{140}$Xe ($Z=54, N=86$) spherical and $^{106}$Mo ($Z=42, N=64$) deformed. This result is in good agreement with experiment [22].

3.2. Nobelium

The results for the $^{252}$No isotope are depicted in Fig 2 where we observe very similar behaviors as the ones encountered in the previous subsection for the Curium isotope. The only relevant differences are the severe reduction of the second fission barrier height that makes very unlikely the existence of a fission isomer and the octupole moment which is substantially smaller. The computed half lives are $4.2 \times 10^5$ s for BCP1 and $3.2 \times 10^{10}$ s for D1S. The $^{252}$No isotope has a half life of 2.44 s with an $\alpha$-decay branching ratio of 66.7%. It decays via SF with a branching ratio of 32.2% and the remaining is electron capture [23]. Therefore the experimental SF half life is 7.2 s which is several orders of magnitude shorter than the computed values. As discussed in the previous section this is not a severe limitation as the impact of triaxiality has not been considered and the $E_0$ parameter has not been used for fine tuning of the SF half lives. What
is relevant is that under the same circumstances, the reduction in the theoretical predictions in going from $^{246}$Cm to $^{252}$No agree very well with the reduction observed in the experimental data. The mass distribution of the fragments corresponds to the isotopes $^{136}$Xe (Spherical) and $^{116}$Cd (slightly deformed) and agrees well with the experimental indications.
3.3. Seaborgium

The results for the $^{270}\text{Sg}$ isotope are depicted in Fig 3 where we observe very similar behaviors as the ones encountered in the previous subsections for the Curium and Nobelium isotopes. For this heavy nucleus the second fission barrier does not exist. The $^{270}\text{Sg}$ isotope has $Z=106$ and $N=164$ and therefore a symmetric split in two $^{135}\text{I}$ will be favored [24] as it implies ending up with magic neutron number $N=82$ in the fragments. We will not study here multimodal fission suggested by the experimental fragment mass distribution and fragment’s kinetic energies. We observe that the octupole moment obtained is zero for the whole quadrupole moment range leading to a symmetric split. The values for the half lives are 5.3 s for BCP1 and 1.2 $10^5$ s for D1S. Again, the Gogny D1S half lives are longer than the ones of BCP1.

4. Conclusions

Fission properties of the BCP EDF have been analyzed in three characteristic examples. The behavior with mass number of the results obtained with BCP1 is similar to the one of the experimental data and other EDFs. We conclude that the BCP EDF is also well suited for the description of fission making broader its range of applicability.

Acknowledgments

Work supported in part by MICINN grants Nos. FPA2009-08958, FIS2009-07277, and FPA2008-03865-E/IN2P3 and by the Consolider-Ingenio 2010 program CPAN CSD2007-00042 and MULTIDARK CSD2009-00064. X. V. also acknowledges the support from FIS2008-01661 (Spain and FEDER) and 2009SGR-1289 (Spain). Support by CompStar, a Research Networking Programme of the European Science Foundation is also acknowledged.

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