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Fission barrier of actinides and superheavy nuclei: effect of pairing interaction

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Abstract. Systematic calculations of fission barriers for axial deformation are performed for even-even nuclei in actinides region of the nuclear chart and superheavy nuclei. These calculations were performed using relativistic Hartree-Bogoliubov (RHB) formalism with separable pairing.

1. Introduction

In the last couple of decades the value of of the height of the inner fission barrier in even-even nuclei has gained a great interest by the nuclear physics community due to its importance to several physics phenomena. For example the formation and stability of super heavy nuclei is determined by the width and height of its fission barrier [1, 2].

Fission barrier, has been studied using covariant density functional theory (CDFT) with different pairing schemes. Inner fission barriers in many nuclei have been calculated in the axially symmetric relativistic mean field (RMF) + BCS approach [3–7]. The authors of [8] showed that the usage of constant gap approximation leads to unphysical results for the fission barriers and suggested that treatment of pairing interaction using effective density-dependent zero-range force is far better approximation of pairing. The authors of [9, 10] used Constant pairing strength in the BCS part, and explored the role of triaxilaity.

In this manuscript a systematic calculations of the fission barriers in the regions of actinides and superheavy of the nuclear chart using relativistic Hartree-Bogoliubov (RHB) theory with sparable pairing formalism. The manuscript is organized as follows; The axial RHB theory with separable pairing and its details related to the calculations of fission barriers are discussed in section 2. The results of the calculation of the fission barriers, and the comparison with experimental data are discussed in section 3. Finally, section 4 summarizes the results of this work.

2. Theoretical framework and the details of numerical calculations

The starting point of Covariant Density Functional Theory (CDFT) is a standard Lagrangian density [11],

$$\begin{aligned}\mathcal{L} \quad &= \bar{\psi}\left(\gamma(i\partial - g_\omega\omega - g_\rho\vec{\rho}\vec{\tau} - eA) - m - g_\sigma\sigma\right)\psi \\ &+\tfrac{1}{2}(\partial\sigma)^2 - \tfrac{1}{2}m_\sigma^2\sigma^2 - \tfrac{1}{3}g_2\sigma^3 - \tfrac{1}{4}g_3\sigma^4 - \tfrac{1}{4}\Omega_{\mu\nu}\Omega^{\mu\nu} + \tfrac{1}{2}m_\omega^2\omega^2 \\ &-\tfrac{1}{4}\vec{R}_{\mu\nu}\vec{R}^{\mu\nu} + \tfrac{1}{2}m_\rho^2\vec{\rho}^2 - \tfrac{1}{4}F_{\mu\nu}F^{\mu\nu}\end{aligned} \tag{1}$$

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where the nucleus consists of point-like nucleons, described by Dirac spinors ψ, interacting via the exchange of mesons with finite masses and leading to the interactions of finite range. The mesons create effective fields in a Dirac equation, which corresponds to the Kohn-Sham equation [12] in the non-relativistic case.

The Lagrangian (1) contains as parameters the meson masses m_σ, m_ω, and m_ρ and the coupling constants g_σ, g_ω, and g_ρ and e is the charge of the protons. The calculations are performed with the NL3* parameterization [13].

$$\begin{aligned}\hat{H}(r) &= \sum_{i=1}^{A}\psi_i(r)^\dagger[\alpha p+\beta m]\psi_i(r)+\frac{1}{2}[(\nabla\sigma)^2+m_\sigma^2\sigma^2+\frac{2}{3}g_2\sigma^3+\frac{1}{2}g_3\sigma^4]-\frac{1}{2}[(\nabla\omega)^2 \\ &+ m_\omega^2\omega^2]-\frac{1}{2}[(\nabla\rho)^2+m_\rho^2\rho^2]+[g_\sigma\rho_s\sigma+g_\omega\gamma_\mu\omega^\mu+g_\rho\vec{j}_\mu\cdot\vec{\rho}_\mu+ej_{p\mu}A^\mu]-\frac{1}{2}[(\nabla A)^2]\end{aligned} \tag{2}$$

Equation (2) represents the Hamiltonian of the nucleus in terms of the mass of the nucleons, mass and the field of the mesons, and the nucleonic density. For details on the theoretical formalism, see [14].

The RHB energy density functional E_{RHB} is given by:

$$E_{RHB}[\hat{\rho},\hat{k}] = E_{RMF}[\hat{\rho}]+E_{pair}[\hat{k}] \tag{3}$$

$E_{RMF}[\hat{\rho}]$ is given by:

$$E_{RMF}[\psi,\bar{\psi},\sigma,\omega^\mu,\vec{\rho^\mu},A^\mu]=\int d^3rH \tag{4}$$

and the $E_{pair}[\hat{k}]$ is given by:

$$E_{pair}[\hat{k}] = \frac{1}{4}\sum_{n_1n_1^{'}}\sum_{n_2n_2^{'}}k^*_{n_1n_1^{'}} < n_1n_1^{'}|V^{PP}|n_2n_2^{'}> k_{n_2n_2^{'}} \tag{5}$$

$< n_1n_1^{'}|V^{PP}|n_2n_2^{'}>$ are the matrix elements of the two-body pairing interaction.

$$\begin{aligned}V^{PP}(r_1,r_2,r_1',r_2') &= -G\delta(R-R')P(r)P(r') \\ R &= \frac{1}{\sqrt{2}}(r_1+r_2) \qquad r=\frac{1}{\sqrt{2}}(r_1-r_2)\end{aligned} \tag{6}$$

$$P(r)=\frac{1}{(4\pi a^2)^{3/2}}e^{-r^2/2a^2} \tag{7}$$

The calculations are performed by imposing constraints on the axial mass quadrupole moment. The method of quadratic constraints uses a variation of the function

$$\left\langle\hat{H}\right\rangle+C_{20}(\langle\hat{Q}_{20}\rangle-q_{20})^2 \tag{8}$$

where $\left\langle\hat{H}\right\rangle$ is the total energy and $\langle\hat{Q}_{20}\rangle$ denotes the expectation value of the mass quadrupole operator

$$\hat{Q}_{20} = 2z^2-x^2-y^2 \tag{9}$$

In these equations, q_{20} is the constrained value of the multipole moment, and C_{20} the corresponding stiffness constant [15].

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3. Results and discussion

3.1. Actinides

A systematic calculations has been performed for even-even nuclei in the actinides region of the nuclear chart, where experimental data exists, allowing only axial deformation. It has been shown in [9] that triaxiality lowers the height of the barrier by $1-4$ MeV, and that the average deviation from experimental data, was around 1 MeV. The axial calculations provide an upper limit on the height of the inner fission barrier. If one looks at the results shown in figure 7 of [9] and extract the values of the inner fission barrier for the axial results, the average deviation between theoretical and experimental results can then be computed. The average deviation would increase by an extra 1.5 MeV and becomes around 2.5 MeV. The average deviation

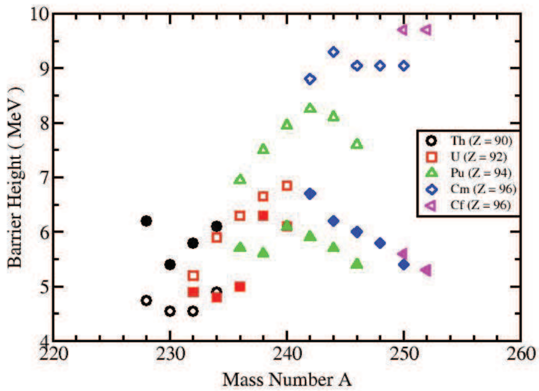

Figure 1. (Color online) Open symbols are the theoretical values of the height of the fission barrier, while filled symbols are the experimental values taken from [16].

between the theoretical and experimental data shown in figure 1 is 1.8 MeV, which is around 30% better than what was obtained in [9]. This result points that the usage of RHB theory with separable paring formalism enhances the description of the fission barrier.

It can be noticed that with the exception of Th isotopes, our calculations over estimate the experimental values of the fission barrier. Our values of the Th isotopes barrier heights is around 4.5 MeV and the experimental data are around 5.5 MeV. However, the trend in the change in the barrier heights as a function of the mass number is similar in both cases. For Pu, Cm and Cf isotopes, our values of the barrier heights is shifted by a constant value from the experimental data. We expect that the inclusion of triaxiality in the calculations would bring our results closer to the experimental data. The major difference comes in the U isotopes, the experimental values are constant in the beginning of the chain then there is a sudden jump. Our results show a steady increases along the chain.

3.2. Superheavy

As mentioned in Sec.3.1 separable pairing perform better than BCS approximation in the pairing channel. It was shown in [10] that triaxiality doesn't affect the height of the inner fission barrier in superheavy region, Z=112-120.

In figure 2, the height of fission barrier for the superheavy nuclei is plotted as a function of the mass number. For Z = 112, one can see that the height of the barrier decreases with the number of neutrons until it reaches a minimum value of 3.5 MeV at N = 168, then it starts to increase to a maximum value of 4.5 MeV. However, this trend is different from the one for Z =

114 and 116 isotopes, where the barrier height increases along the isotopic chain. It starts from 4 MeV up to 5 MeV for Z = 114, and from 4 to 5.5 MeV in Z = 116 For Z = 118, the results

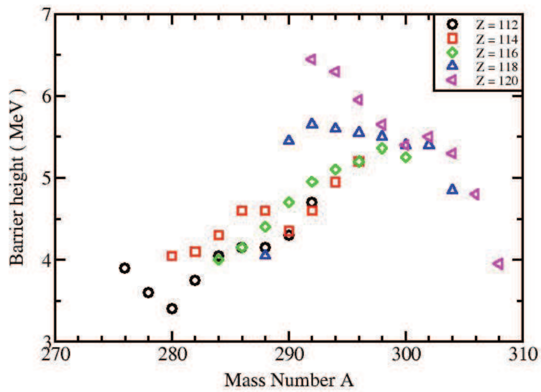

Figure 2. (Color online) Height of inner fission barrier for superheavy nuclei.

show a constant value of the fission barrier, and then it starts to decrease around A = 300. In Z = 120 chain, the highest value of the barrier is obtained for A = 292, which corresponds to N = 172. $^{292}120$ (292 is the mass number and 120 is the proton number) is known to be spherically doubly magic, and thus it is expected to have the highest fission barriers among the nuclei in that region. The difference between the largest and smallest value is around 3 MeV.

4. Conclusion

Systematic calculation of the fission barrier in two regions; actinides and superheavy, using RHB theory with separable pairing formalism has been performed. It is been demonstrated, when only axial deformation is allowed, that RHB theory with separable pairing perform better than RMF+BCS. The average deviation of the height of the fission barrier is reduced by 30% as compared with the results obtained in [9]. The height of the inner fission barrier in superheavy nuclei was also calculated.

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