Calculation of Q_α in heavy and superheavy nuclei*

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The study of alpha decay of heavy and superheavy nuclei is of key relevance to traceback the synthesis of new elements in the laboratory. In addition, this process plays an important role in the late stages of r-process nucleosynthesis calculations. However, a limited experimental information is available nowadays and reliable theoretical descriptions are already required. Energy density functional methods are currently the only theoretical approach to calculate microscopically properties of heavy and superheavy nuclei [1]. These methods are based on self-consistent mean field (MF) approximations such as the Hartree-Fock-Bogoliubov (HFB) one [2]. In spite of its simplicity, the HFB approach has proved to be successful in describing bulk properties of the atomic nuclei. However, some important correlations related to the symmetry restorations and quantum fluctuations cannot be accounted by the HFB approximation and one has to go beyond mean field (BMF) to get a better description of the system [1]. In this contribution we discuss an example of MF and BMF calculations of the Q_α-value in the plutonium isotopic chain using the Gogny D1M parametrization [3]. This quantity is defined as $Q_\alpha(A) = B.E.(^4\mathrm{He}) + B.E.(^{A-4}\mathrm{U}) - B.E.(^A\mathrm{Pu})$, where A and $B.E.$ are the mass number and the nuclear binding energy respectively.

We first analyze the convergence of the HFB calculations with the size of the spherical harmonic oscillator basis in which the HFB states are expanded [2]. In Fig. 1(a) the Q_α-values obtained for different number of major oscillator shells, $N_{h.o.}$, included in the MF calculation are represented. We observe the curves approaching each other with increasing $N_{h.o.}$ showing a nice convergence pattern. However, the fully converged HFB result is not able to reproduce the experimental data. In addition, the calculations are not fully converged for the lighter nuclei $N \in (138-146)$ using $N_{h.o.} = 12$, having Q_α differences up to 0.5 MeV with respect to the values obtained with $N_{h.o.} = 18$.

We can also explore at the MF level the role of octupole deformations (β_3) in the Q_α-values. In Fig. 1(b) the results of the calculations including or not this degree of freedom are represented. We see differences only in the three lightest nuclei and, surprisingly, the theoretical results with $\beta_3 = 0$ are in better agreement with the experiment. However, this is an artifact either from the interaction and/or from the lack of parity projection that must be further investigated.

Finally, we analyze the effect of including angular momentum and particle number restoration, plus axial quadrupole shape mixing (GCM method) in the Q_α-values calculated here. In this case, we have two additional important limitations: 1) only parity conserved HFB wave functions ($\beta_3 = 0$) are included, and, 2) we have used $N_{h.o.} = 12$ due to the large computational cost, although we have already discussed that the results are not fully converged. Nevertheless, it is important to study which are the changes introduced by these correlations in this particular example. Most of the nuclei calculated here are deformed and superfluid. Hence, both angular momentum and particle number restoration provide ~ 4 MeV and configuration mixing gives ~ 1 MeV of extra binding energy. However, this energy gain is not completely constant along the isotopic chain and depends on the underlying subshell structure of each nuclei. In Fig. 1(c) we show that the results are indeed quite sensitive to BMF effects, particularly from $N = 138-148$. However, artificial jumps in $N = 138$ and $N = 148$ are obtained and must be further investigated.

In summary, we have shown the Q_α-value calculation for plutonium isotopic chain using energy density functional methods with the Gogny D1M parametrization. We have observed that the results are very sensitive (up to ~ 1 MeV) to the convergence of the method, the inclusion of collective degrees of freedom such as octupole deformation, and beyond mean field effects. These uncertainties require further analysis and work is in progress to provide reliable theoretical results in the near future.

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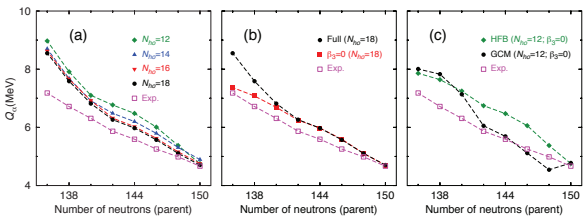

Figure 1: Q_α for the Pu chain calculated with the Gogny D1M interaction: (a) for different values of the oscillator shells included in the HFB calculation, (b) allowing octupole deformations (bullets) or not (filled squares) in the HFB states ($N_{ho} = 18$), (c) with plain HFB (bullets) or including BMF effects (filled squares) ($N_{ho} = 12$, $\beta_3 = 0$). Open squares are the experimental values.

References

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