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Gogny-HFB convergence analysis and Beyond-Mean-Field correlations*

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Introduction

r-Process stellar nucleosynthesis requires accurate predictions of nuclear properties for nuclei far beyond reach of current experimental facilities. Regardless of the potential astrophysical site, the final elemental abundances are very sensitive to the employed global nuclear mass table [1]. Mean-field approaches based on Hartree-Fock-Bogolyubov (HFB) formalism are as microscopic as possible for global calculations, and thus are expected to be more reliable predicting unknown nuclei. However, in order to further increase predictive power of HFB-based models particular attention must be paid to the following three main issues of the currently used HFB-models.

I. Convergence

Ideally, computed observables should be independent of chosen harmonic oscillator (HO) basis, i.e. *converged*. However, due to basis truncation, and asymptotic behavior of HO–functions, calculations for heavy and/or neutron-rich systems are generally *not fully converged*.

A better treatment of convergence in our global survey [2] of 2180 even-even nuclear masses up to the drip lines based on Gogny-D1S HFB approach noticeably improved agreement with experimental data: *(a)* when compared with the previously published database [3] our results are better converged by ∼1.5 MeV; *(b)* the root-mean-square (rms) deviation from the 594 experimental masses in AME12 compilation [4] is reduced from 4.6 MeV to 3.5 MeV with the most sizeable improvement in-between the shell closures; *(c)* numerical noise due to lack of convergence is removed, resulting in smoother two-neutron separation energies for every isotopic chain.

Evident lack of convergence prompted us to perform systematic studies of two recently proposed energy correction schemes: empirical MVS–A [5] and theoretically justified L_{eff}–extrapolation [6]. Unfortunately none of them provide reliable and consistent results for r-process nuclei [7].

II. Beyond-Mean-Field (BMF) Correlations

A significant improvement in precision of HFB models is expected after including the BMF corrections, such as *(i)* particle number, and *(ii)* angular momentum projections, as well as *(iii)* configuration mixing. Because of high computational cost, all pioneer global BMF–surveys using generator coordinate method (GCM) were carried out assuming the so called Gaussian overlap approximation (GOA). We performed global calculation with the mentioned D1S and an improved Gogny-D1M parametrization using the exact implementations of GCM methods assuming axial symmetry. Our results [8] show: *(a)* BMF–effects amount to 5–6 MeV of correlation energy; *(b)* as in all published mass–tables, the BMF–corrections decrease the scatter in the computed masses, especially for light nuclei; *(c)* the neutron and proton shell gaps at N and Z =20, 28 are also slightly reduced, but we do not see the reported previously [3, 9] shell quenching for the remaining shell gaps.

III. Odd-Even Effects

Description of odd-mass isotopes within the same HFB approach requires time-reversal symmetry breaking, which makes computation task an order of magnitude more expensive. In order to make global calculation for all isotopes feasible, we had to employ perturbative nucleon addition method, which inevitably leads to uncertainties, such as *(i)* gradually increasing overestimation of neutron separation energies in vicinity of N-shell closure, and *(ii)* largely exaggerated shell gap. Further investigations of this approximation, as well as possibilities of other methods are the topics of our current research.

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* **AA** is supported by the Helmholtz Association through Nuclear Astrophysics Virtual Institute (NAVI), VH-VI-417. **TRR** was supported from the BMBF-Verbundsforschungsprojekt number 06DA7047I. **GMP** acknowledges support by the Deutsche Forschungsgemeinschaft through contract SFB 634 and the LOEWE program launched by the state of Hesse. The calculations were performed on the CPU supercomputer cluster LOEWE-CSC of Goethe University Frankfurt, and PROMETHEUS cluster of the computing facility at GSI Helmholtz Centre for Heavy Ion Research (GSI).

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DOI:10.15120/GR-2015-1-MU-THEORY-10