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Convergence properties of density-matrix expansions

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One of the current projects at the Department of Physics in the University of Jyväskylä is to explore more general forms of the Skyrme energy-density functional (EDF). The aim is to find new phenomenological terms which are sensitive to experimental data.

In this context we have extended the Skyrme functional by including terms which contain higher orders of derivatives allowing for a better description of the long range part of the nuclear force. This was done by employing an expansion in derivatives in a spherical-tensor formalism [1] motivated by ideas of the density-matrix expansion (DME). If the expansion coefficients are treated as free parameters the resulting functionals gets different number of free parameters depending on the order in derivatives and assumed symmetries. The usual Skyrme EDF is obtained as a second order expansion while we keep terms up to the sixth order.

The resulting self-consistent mean-field equations as well as the linear-response equations can be derived straightforwardly in a systematic way and solved using computer codes [2].

This formalism and code are used to evaluate different expansions of the non-local density. As an example the Hartree-Fock energy from the Gogny force is considered and the exact energy is compared with the energy obtained when using DMEs. Starting from a force in this way, all the free parameters in the functional can be derived so that the total energy becomes a functional of the local density and its derivatives which is much faster to use than the full exchange term. A new DME method is also presented which is more accurate than previous versions.

Methods based on the DME constitute a natural first step towards obtaining an ab-initio universal energy density functional which is able to give accurate and reliable descriptions of low-energy observables for the medium-to-heavy exotic nuclei studied at the new experimental facilities. This work constitutes the first test of convergence properties of different DMEs which are considered up to the sixth order.

[1] B.G. Carlsson, J. Dobaczewski, and M. Kortelainen, Phys. Rev. C 78, 044326 (2008)
[2] B.G. Carlsson, J. Dobaczewski, J. Toivanen and P. Vesely, submitted to Comp. Phys. Comm., arXiv:0912.3230v1 [nucl-th] (2009)

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