Regularization of Multi-Reference Energy Density Functional Calculations

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Being based on symmetry-breaking "intrinsic" configurations is one of the key features for the descriptive and explanatory sucesses of the self-consistent mean-field method [1]. This allows to model a large part of multipole, pairing, and some other correlations in finite nuclei in a very efficient manner. It is, however, often desirable to restore the broken symmetries, which then adds further correlations to the model and re-establishes the quantum numbers of the many-body states and selection rules for transitions between them. Exact symmetry restoration requires to use a multi-reference framework in the spirit of the Generator Coordinate Method (GCM). The same framework allows also for the description of fluctuations in collective degrees of freedom. Nowadays, there are several groups using models that combine symmetry restoration and shape mixing based on self-consistent mean-field models and using an energy density functional methods as effective interaction [2]. Recently [3], however, it has been pointed out that using the standard procedure to calculate the non-diagonal kernels of the energy functional introduces spurious terms that, for example, might lead to divergencies, steps or other discontinuities when the projected energy is plotted as a function of a collective coordinate. In Refs. [3-6], the appearance of these discontinuities was identified to be the consequence of one of an implicit choice made when extending the energy density functional to multi-reference calculations. Indeed, in Refs. [4,5] it could be shown that he standard procedure that uses an analogy with a generalized Wick theorem multiplies small unphysical spurious contributions to the energy that are present in all energy functionals, which do not correspond to a Hamilton operator, with unphysical weights that might become very large. As pointed out in Ref. [4], there are alternative procedures to calculate the non-diagonal energy kernels, at least for certain classes of functionals [6], which are free of discontinuities without modifying the physical contribution to the energy functional [5]. Examples for calculations with such regularized energy functionals will be presented, and consequences for the design of future energy functionals discussed.

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