Instabilities in the Nuclear Energy Density Functional

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Abstract. In the field of Energy Density Functionals (EDF) used in nuclear structure and dynamics, one of the unsolved issues is the stability of the functional. Numerical issues aside, some EDFs are unstable with respect to particular perturbations of the nuclear ground-state density. The aim of this contribution is to raise questions about the origin and nature of these instabilities, the techniques used to diagnose and prevent them, and the domain of density functions in which one should expect a nuclear EDF to be stable.
The Energy Density Functional (EDF) method is a broadly used tool in the study of nuclear structure and dynamics, allowing to describe medium-mass to heavy nuclei with reduced computational cost. This is achieved thanks to the implicit resummation of quantum many-body correlations into an effective energy functional of local densities, which is, in principle, minimized for the intrinsic density of the many-body ground state (i.e. the density in the center-of-mass frame \cite{1}, possibly breaking several symmetries of the Hamiltonian). Non-relativistic EDFs mostly used in nuclear physics until now are of the Skyrme type, i.e. semi-local functionals with a postulated analytical form and no clear connection to the “bare” two- and three-nucleon interactions.

The Skyrme EDF has been employed not only in static “mean-field” calculations, but also for the study of small- or large-amplitude collective dynamics in schemes such as Time-Dependent-Hartree-Fock (TDHF), or Quasiparticle Random-Phase Approximation (QRPA). Furthermore, the power of the Multi-Reference EDF method \cite{2, 3}, which includes collective-motion correlations into ground and excited states through the resolution of the Hill-Wheeler equations, has been thoroughly demonstrated.

In the present article we concentrate on “Skyrme-like” or semi-local functionals. One of the intrinsic, unsolved issues of these functionals is the stability and convergence of calculations performed with them. Besides numerical issues linked with finding an energy minimum, especially a constrained one, some functionals appear unstable with respect to specific perturbations of the nuclear density. This instability means that self-consistent calculations will yield unphysical configurations at energy minimum, break symmetries expected in the minimum-energy density (i.e. other than those supposed to be explicitly broken such as spherical symmetry) and/or yield a divergent energy. This is now understood to be an intrinsic defect of some functionals, independently from numerical details \cite{1, 5}.

The Skyrme EDF can be expressed through the local energy density $\mathcal{H}$,

$$\mathcal{H} = \frac{\hbar^2}{2m} t_0 + \mathcal{H}_0 + \mathcal{H}_1,$$

where isoscalar ($t = 0$) and isovector ($t = 1$) terms have been separated; both have the same structure, i.e. for even-even nuclei,

$$\mathcal{H}_t = C^\rho_t \rho_t^2 + C^\tau_t \rho_t \tau_t + C^{\Delta \rho}_t \rho_t \Delta \rho_t + C^{\nabla J}_t \rho_t \nabla J_t + C^J_t J_t^2,$$

where $\rho$, $\tau$, and $J$ are respectively the matter, kinetic, and spin-current densities, an index $t = 0,1$ indicating respectively isoscalar and isovector quantities; standard definitions of the latter can be found in Refs. \cite{1, 6}. In typical Skyrme parametrizations, density dependence is introduced as $C^\rho_t = C^\rho_0 + C^\rho_{1D} \rho_0$, with $\rho_0 = \rho_n + \rho_p$. Generalizations involving a dependence of coupling constants on the isovector density $\rho_1 = \rho_n - \rho_p$ and/or more involved functions of densities are being studied. Recent work \cite{7, 8} aiming at building non-empirical, yet semi-local, functionals through the Density Matrix Expansion (DME) method \cite{9} also leads to such generalized forms.

The instability of Infinite Nuclear Matter (INM) and nuclei with respect to global spin and/or isospin polarization is a common problem for functionals derived strictly
as the expectation value of a Skyrme effective interaction, and has been repeatedly discussed and addressed \cite{10, 11, 12}. However, these pathologies of the INM Equation of State (EOS), usually occurring at high densities, hardly affect nuclear structure calculations in practice.

More recently, a divergence of the total energy and densities has been observed in EDF calculations of finite nuclei \cite{4} performed with specific parameterizations of the Skyrme functional \cite{13, 14}. Fig. 1 displays densities obtained with these parameterizations in two sample nuclei at various (large) numbers of iterations of the self-consistent equations. Characteristic traits of this phenomenon include unnatural configurations (large-amplitude spatial oscillations of densities, with separation of protons and neutrons) and unnaturally large (negative) total energy. This instability was analyzed by studying the response of INM, used as a model system, to finite-size density perturbations at the Random Phase Approximation (RPA) level.

When calculated with the central terms of the residual interaction deduced from a semi-local functional \cite{16}, the analytic expressions for the RPA response functions are rather involved, even more so when the spin-orbit \cite{17} and tensor \cite{18} terms are added. For the sake of discussion, it is useful to consider the case of a functional with $C_t^r = C_t^J = C_t^{\nabla J} = 0$ (which is strictly local, despite the remaining $\rho \Delta \rho$, “finite-range” terms) considering isospin density fluctuations only. One then finds the textbook result.
for the response function in symmetric INM,

$$\Pi(\omega, \mathbf{q}) = \frac{4 \Pi_0(\omega, \mathbf{q})}{1 - 8 [C_1^\rho - C_1^\Delta \rho \mathbf{q}^2] \Pi_0(\omega, \mathbf{q})}$$  \hspace{1cm} (3)$$

where $\omega$ is the excitation energy, $\mathbf{q}$ the transferred momentum, or wave number of the density fluctuation, $\Pi(\omega, \mathbf{q})$ the response function, and $\Pi_0(\omega, \mathbf{q})$ the non-interacting response, or Lindhard function [19]. The value $\Pi(\omega = 0, \mathbf{q})$ corresponds to the static susceptibility of the system to finite-size perturbations. It should be positive (with the above sign convention) for all values of $\mathbf{q}$ and the density $\rho_0$. (We recall that the coupling constants in the above equation can depend on the latter, as does $\Pi_0$.) A change of sign with either variable is accompanied by a pole signaling the existence of a zero-energy collective mode. We see that the short-wavelength (high $\mathbf{q}$) behaviour is driven by the coefficient $C_1^\Delta \rho$, whose value correlates with the occurrence rate of the instability observed in calculations of finite nuclei [4]. A similar convergence issue was identified in Ref. [20], and confirmed in Ref. [5], concerning the susceptibility of the functional SkO [21] to fluctuations of the spin density.

We could categorize these instabilities in terms of the importance and role of the finite size of the system under consideration. First of all, Landau’s theory of Fermi fluids [22] gives quantitative constraints for the stability vs. long-range perturbations of INM in terms of Landau parameters. Second, the more general random-phase approximation (RPA) calculations in INM can, at least qualitatively, link zero-energy modes to oscillations of densities in static calculations of nuclei. Third, in finite nuclei, instabilities originating at the surface may not be amenable to a diagnosis through INM calculations. This may be emphasised, in particular, by the recent attention brought to more involved density dependences [23]. This leads to ask a first open question:

1 Can we quantitatively understand the link between instabilities in INM and finite nuclei? In particular, what INM densities are relevant to the study of nuclei? How does finite size modify the results from INM?

The principal manifestation of instabilities described up to now seems to be divergence of given quantities. However, let us point out that this is not mandatory for a functional to exhibit unstable behaviour. A schematic representation of the EDF energy with respect to an abstract collective coordinate $x$ in the EDF calculation (e.g. in Fig. 1 the magnitude of the density oscillations) is given in Fig. 2. Here the dot at $x = 0$ represents the physically expected configuration. Curve (a) corresponds to the (desired) situation with a stable configuration, whereas curve (d) represents a well-developed instability. Curves (b) and (c) represent situations with a metastable minimum which can be made to evolve to more energetically favored configurations by some perturbation. In case (b) a true, global variational solution exists; whereas in case (c) it does not. Here, RPA (i.e. linear response) analysis would only warn about situation (d).

Case (b) was encountered in Appendix B of Ref. [24], where a parameterization with large negative values of $C_1^\rho$ was found to yield, in seemingly random nuclei, an unphysical shell structure. The plot of the energy landscape as a function of the magnitude of the
Figure 2. Schematic picture of energy landscape with respect to collective coordinate $x$, assumed to be constrained while other degrees of freedom are variationally optimized, for stable (a) and various unstable cases. See text.

spin-current density $J$ in Fig. 35 of Ref. [24] indeed corresponds quite well to case (b), with two minima, the unphysical one being energetically favored. Thus, it seems appropriate to ask:

2 How can we diagnose instabilities not accessible with a small-amplitude expansion around the expected ground state (as in RPA)?

In Ref. [25], a TDHF calculation of a central $^{16}$O-$^{16}$O reaction done with the functional SkM$^*$ [26] showed that after contact, the two nuclei separated exhibiting a toroidal spin polarization. This puzzling result might be analyzed from the standpoint of stability analysis: is this configuration lying lower in energy than a more “reasonable” one? If so, this result might well have to be discarded. It is also possible that a treatment beyond the static considerations above (i.e. referring to energy minimization) be necessary for a thorough understanding, and hence:

3 What are the manifestations of instabilities developing on top of excited states, probed in dynamical calculations? Can we reduce their study to a model problem, such as the INM analysis above?

Finally, current efforts tend towards producing non-empirical semi-local functionals through the DME applied to low-momentum interactions [27]. The DME, more than a simple range expansion, consists of a series of finite-size corrections to the INM density matrix [9, 7, 8]. It can thus be expected to be accurate for smoothly varying densities such as those occurring naturally in nuclei. However, there is no guarantee that this accuracy will be preserved for pathologic configurations such as in Fig. [1]. In other words, extra care should be taken to verify that the DME functional does not exhibit pathological behaviour beyond its expected domain of validity. Indeed, by going from an exact Hartree-Fock functional deduced from a realistic Hamiltonian to a semi-local functional, spurious high-momentum components are introduced e.g. in the residual interaction and response functions (Eq. (3)). The apparent link between RPA linear
response analysis and self-consistent EDF calculations suggests that the “singularity” due to the semi-local nature of the functional can make divergences, naturally expected in calculations beyond first order of perturbation theory performed with a zero-range interaction, creep into “mean-field” ones through self-consistency. Our final question is thus:

4 How far in density should we expect the next-generation nuclear EDF to be stable, and in what domain of variation for the reference Slater determinant and associated densities? In other words, shouldn’t semi-local functionals be specified with a well-defined “cutoff” or resolution scale?

It is especially important to understand this issue for functionals containing higher-order derivative terms (yielding higher orders of $q$ in Eq. (3)) such as proposed in Ref. [28], whether they are built from an underlying Hamiltonian or purely phenomenological.

In summary, despite their great usefulness, semi-local nuclear energy density functionals of the Skyrme type come with several kinds of stability-related issues, which can compromise the significance of results obtained with them. Indeed, whereas in the process of developing new nuclear functionals, one naturally focuses on minimum (ground-state) energies and associated density configurations, these functionals will be probed in different ways in actual applications, be it during energy minimization or in dynamical extensions of the theory. These issues should thus be fully understood and kept in mind for future development.

Acknowledgements

We acknowledge fruitful discussions with M. Stoitsov and N. Schunck. This work was supported by the U.S. Department of Energy under Contract Nos. DE-FG02-96ER40963, DE-FC02-07ER41457, DE-FC02-09ER41583 (UNEDF SciDAC Collaboration), and DE-FG02-07ER41529 (University of Tennessee).

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