Performing safe multi-reference energy density functional calculations

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Configuration mixing calculations performed in terms of Skyrme, Gogny or relativistic Energy Density Functionals (EDF) rely on extending the Single-Reference energy functional into non-diagonal EDF kernels. The standard prescription to do so, based on an analogy with a Hamiltonian theory and the use of the generalized Wick theorem, is responsible for the recently observed divergences and steps in Multi-Reference calculations. We summarize the minimal solution to this problem recently proposed [1] and applied with success to particle number restoration [2]. Such a regularization method provides suitable corrections for EDF depending on integer powers of one-body density matrices only. The specific case of fractional powers of the density [3] is also briefly discussed.

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I. ENERGY DENSITY FUNCTIONAL METHODS

The nuclear Energy Density Functional (EDF) method is a unique tool to study static and dynamical properties of nuclei in a unified framework [4]. Although the nuclear EDF shares several features with Density Functional Theory [5] (DFT), the strategy used is different as it embraces two successive levels of description.

On the first level, traditionally called "self-consistent mean-field theory", Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB), a single product state Φ_0 provides the normal ρ^{00} and anomalous κ^{00} density matrices the many-body energy is a functional of. We call this method a single-reference (SR) EDF approach and denote by $\mathcal{E}_{SR}[\Phi_0] = \mathcal{E}_{SR}[\rho^{00}, \kappa^{00}, \kappa^{00\,*}]$ the actual EDF. Although such a restriction is not necessary, one usually builds the EDF from an auxiliary effective vertex (of the Skyrme or Gogny type) or an auxiliary effective Lagrangian, whose parameters are adjusted to reproduce a selected set of experimental observations. Independently of the starting point, the EDF can be written in any arbitrary basis as

$$\begin{aligned}\mathcal{E}_{SR}[\rho^{00}, \kappa^{00}, \kappa^{00\,*}] \;=\; & \sum_{ij} t_{ij}\, \rho^{00}_{ji} + \frac{1}{2}\sum_{ijkl} \bar{v}^{\rho\rho}_{ijkl}\, \rho^{00}_{ki}\, \rho^{00}_{lj} + \frac{1}{4}\sum_{ijkl} \bar{v}^{\kappa\kappa}_{ijkl}\, \kappa^{00\,*}_{ij}\, \kappa^{00}_{kl} \\ & + \frac{1}{6}\sum_{ijklmn} \bar{v}^{\rho\rho\rho}_{ijklmn}\, \rho^{00}_{li}\, \rho^{00}_{mj}\, \rho^{00}_{nk} + \frac{1}{4}\sum_{ijklmn} \bar{v}^{\rho\kappa\kappa}_{ijklmn}\, \rho^{00}_{li}\, \kappa^{00\,*}_{jk}\, \kappa^{00}_{mn} + \dots \;,\end{aligned} \tag{1}$$

where the first term accounts for the uncorrelated kinetic energy, whereas $\bar{v}^{\rho\rho}$, $\bar{v}^{\kappa\kappa}$, $\bar{v}^{\rho\rho\rho}$, ... denote effective vertices associated with the different terms of the EDF. There are a few important comments to be made at this point. First, and although it formally resembles it, Eq. (1) should not be confused with the expectation value of a Hamiltonian containing two-body, three-body, ... interactions in the Hartree-Fock-Bogolyubov state Φ_0. For this to be true, specific properties, e.g. $\bar{v}^{\rho\rho}_{ijkl} = \bar{v}^{\kappa\kappa}_{ijkl}$ and $\bar{v}^{\rho\rho}_{ijkl} = -\bar{v}^{\rho\rho}_{ijlk}$ for all (i, j, k, l), would have to be satisfied, which is usually not the case in the EDF context. Second, most popular and high-performance EDF

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cannot be written under the form of Eq. (1) as they contain a dependence on a non-integer power of the (local) normal density [4]. We anticipate, however, that future EDFs will be constructed under such a form, typically truncated at forth or fifth power. Indeed, the regularization procedure presented here is inapplicable to EDFs containing non-integer powers of the density matrices [3].

While static collective correlations, e.g. pairing and deformation, can be accounted for within the SR EDF formalism through the symmetry breaking of the auxiliary state Φ_0, including dynamical collective correlations associated with collective quantum fluctuations requires to perform a so-called Multi-Reference (MR) calculations, traditionally denoted as "beyond-mean-field". Such an extension, built by analogy with the Generator Coordinate Method (GCM) in the Hamiltonian formalism [6], allows one not only to incorporate additional correlations but also to describe low-energy spectroscopy and transition probabilities between states characterized by symmetry-restored quantum numbers. In strict analogy with the Hamiltonian formalism, the MR EDF is written as

$$\mathcal{E}[\Psi] \equiv \frac{\sum_{\{0,1\}\in \mathrm{MR}} f_0^* \, f_1 \; \mathcal{E}_{MR}[\Phi_0,\Phi_1] \, \langle \Phi_0 | \Phi_1 \rangle}{\sum_{\{0,1\}\in \mathrm{MR}} f_0^* \, f_1 \, \langle \Phi_0 | \Phi_1 \rangle} \quad , \tag{2}$$

where non-diagonal matrix elements $\langle \Phi_0 | \hat{H} | \Phi_1 \rangle / \langle \Phi_0 | \Phi_1 \rangle$ have been replaced by their EDF counterpart $\mathcal{E}_{MR}[\Phi_0, \Phi_1]$. The weight functions f are determined either by symmetry considerations, by diagonalization, or both depending on the MR modes included in the calculation. The product states Φ_i belonging to the MR set are chosen according to the collective modes one wants to describe. In the absence of a well-founded prescription to build $\mathcal{E}_{MR}[\Phi_0, \Phi_1]$, only specific constraints can be imposed. For a number of reasons [7], it is necessary to impose that $\mathcal{E}_{MR}[\Phi_0, \Phi_0] \equiv \mathcal{E}_{SR}[\Phi_0]$ and $\mathcal{E}_{MR}[\Phi_1, \Phi_0] = \mathcal{E}^*_{MR}[\Phi_0, \Phi_1]$. Following the Hamiltonian formalism, the most natural guidance is provided by the generalized Wick theorem [8] (GWT) which suggests that $\mathcal{E}_{MR}[\Phi_0, \Phi_1]$ is obtained by replacing SR density matrices by transition ones, i.e. $[\rho^{01}, \kappa^{01}, \kappa^{10\,*}]$, in Eq. (1). However, we have shown that the use of GWT-based functional energy kernels is the source of the pathologies recently

observed in MR-EDF calculations [1–3].

A. Pathologies observed in configuration mixing calculations

An example of deformation energy surface obtained through a MR calculation based on Particle-Number Restoration (PNR) is given for ^{18}O in the left panel of Fig. 1 using the SLy4 Skyrme EDF together with a density-dependent zero-range pairing interaction. Starting from the SR-EDF built from the auxiliary state Φ_0 that breaks the gauge symmetry associated with particle-number conservation, dynamical pairing correlations associated with PNR can be incorporated through a MR EDF calculation. Building the MR set from product states rotated in gauge space $|\Phi_\varphi\rangle = e^{i\varphi\hat{N}}|\Phi_0\rangle$, Eq. (2) specified to PNR reads [1]

$$\mathcal{E}^N \equiv \int_0^{2\pi} d\varphi \, \frac{e^{-i\varphi N}}{2\pi \, c_N^2} \, \mathcal{E}_{MR}[\Phi_0, \Phi_\varphi] \, \langle \Phi_0 | \Phi_\varphi \rangle \, . \tag{3}$$

In practice, Eq. (3) is numerically calculated using the Fomenko [10] discretization procedure. Figure 1 presents results obtained for two different numbers of mesh points in the discretization (dotted and dashed lines). Obvious pathologies are visible, i.e. (i) the estimate of the energy landscape does not converge and (ii) non-physical steps and divergencies appear at particular deformations as one increases the number of mesh points used in the Fomenko procedure. Authors have not only faced the problem for PNR [11, 12] but also in angular-momentum restoration calculations [13]. As visible in Fig.1, it has been recognized [11] that divergences in PNR may appear when either a proton or neutron single-particle level crosses the Fermi en energy, as pair of states differing by $\pi/2$ are orthogonal in this case, i.e. $\langle \Phi_0 | \Phi_\varphi \rangle = 0$. When the same (density-independent) vertices are used in the p-h and p-p channel and the exchange is properly taken into account, problems do not appear. The problem has been characterized more precisely thanks to a complex plane analysis [14], demonstrating in particular the less obvious but more profound occurrence of finite steps. The latter analysis could not, however, lead to a practical solution of the problem.

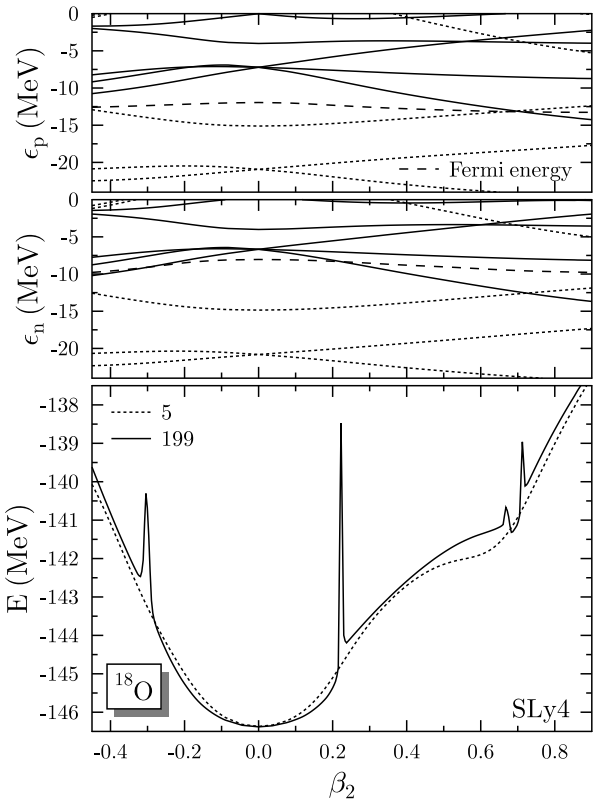

FIG. 1: Particle-number restored deformation energy surface of ^{18}O calculated with SLy4 and a density-dependent pairing interaction and the corresponding single-particle spectra of protons and neutrons as a function of the axial quadrupole deformation for $L = 5$ and 199 discretization points of the integral over the gauge angle (lowest panel).

II. MINIMAL SOLUTION TO THE PROBLEM

We have recently shown that the origin of those difficulties can be traced back to the strategy used to design energy kernels entering the MR-EDF, i.e. the use of the GWT as a guidance. An early hypothesis [11], confirmed later on [12], was that problems could be avoided in PNR calculations by using another prescription than the one based on the GWT to defined the non-diagonal energy kernels. More recently, this idea has been used to design a general solution that applies to any type of MR mode [1]. The technique makes use of the following trick: given a pair of quasi-particle vacua, denoted by $|\Phi_0\rangle$ and $|\Phi_1\rangle$ (with possibly $\langle\Phi_0|\Phi_1\rangle = 0$), one

can always find a simple "BCS like" expression connecting these two states, i.e. [6]:

$$|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod_{p>0} \left(\bar{A}^*_{pp} + \bar{B}^*_{p\bar{p}}\, \tilde{\alpha}^+_p\, \tilde{\alpha}^+_{\bar{p}}\right) |\Phi_0\rangle \ . \tag{4}$$

In the canonical quasi-particle basis where Eq. (4) is valid, GWT-based energy kernels read, e.g. for a strictly bilinear EDF, as (omitting the kinetic term)

$$\begin{aligned}
\mathcal{E}_{MR}[\Phi_0,\Phi_1] =& \frac{1}{2}\sum_{\nu\mu} \bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\varphi_\nu\varphi_\mu} + \frac{1}{4}\sum_{\nu\mu} \bar{v}^{\kappa\kappa}_{\varphi_\nu\phi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}} && (5)\\
&+\frac{1}{2}\sum_{\nu\mu} \bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\varphi_\mu}\, \bar{Z}_{\nu\bar{\nu}} + \frac{1}{4}\sum_{\nu\mu} \bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}}\, \bar{Z}_{\nu\bar{\nu}} && (6)\\
&+\frac{1}{2}\sum_{\nu\mu} \bar{v}^{\rho\rho}_{\varphi_\mu\varphi_\nu\varphi_\mu\phi_\nu}\, \bar{Z}_{\nu\bar{\nu}} + \frac{1}{4}\sum_{\nu\mu} \bar{v}^{\kappa\kappa}_{\varphi_\mu\phi_{\bar{\mu}}\phi_\nu\phi_{\bar{\nu}}}\, \bar{Z}_{\nu\bar{\nu}} && (7)\\
&+\frac{1}{2}\sum_{\nu\mu} \bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\phi_\mu}\, \bar{Z}_{\nu\bar{\nu}}\, \bar{Z}_{\mu\bar{\mu}} + \frac{1}{4}\sum_{\nu\mu} \bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\phi_\mu\phi_{\bar{\mu}}}\, \bar{Z}_{\nu\bar{\nu}}\, \bar{Z}_{\mu\bar{\mu}}\ , && (8)
\end{aligned}$$

where $(\mu,\bar{\mu})$ denote a canonical pair in the specific quasi-particle representation, $\bar{Z}_{\bar{\nu}\nu} = (\bar{B}_{\bar{\nu}\nu}/\bar{A}^{-1}_{\nu\nu})^*$ while φ_ν and ϕ_μ stand for the upper and lower components of the quasi-particle states [1]. Expressions (5-8) allow one to understand the origin of the spurious steps and divergences. As the energy kernel is multiplied by $\langle\Phi_0|\Phi_1\rangle \propto \prod_\nu \bar{A}^*_{\nu\nu}$ in the MR energy (see Eq. (2)), terms with $\nu=\mu$ or $\nu=\bar{\mu}$ in line (8) can lead to divergences and steps when $\bar{A}^*_{\nu\nu}=0$. In the pure Hamiltonian case, i.e. $\bar{v}^{\rho\rho}_{ijkl} = \bar{v}^{\kappa\kappa}_{ijkl}$ and $\bar{v}^{\rho\rho}_{ijkl} = -\bar{v}^{\rho\rho}_{ijlk}$ for all (i,j,k,l), the dangerous contributions coming from the two terms in Eq. (8) exactly cancel out and no divergence or step occurs. However, when different or non-antisymmetrized vertices are used, as in the EDF context, divergences and/or steps are observed, as seen on the left panel of Fig. 2 for PNR. The fact that the spurious terms that should cancel out in Eqs.(5-8) generates finite steps can be understood thanks to the complex plane analysis [14].

The quasi-particle basis introduced above allows one to use the standard Wick theorem in the Hamiltonian formalism. By analogy, one can thus define a new extension procedure to define non-diagonal energy kernels that is free from any of the problems discussed above. Indeed, comparing the results of the two schemes, one proves [1] that terms with $\nu=\mu$ or $\nu=\bar{\mu}$ in line (8) should be zero in the

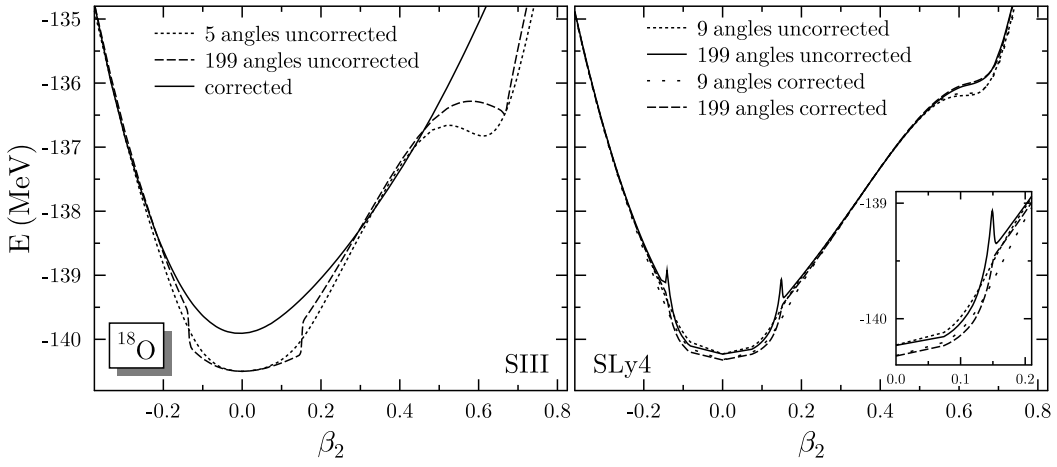

FIG. 2: Left: Uncorrected (dotted and dashed lines) and corrected (solid line) particle-number restored quadrupole deformation energy obtained for ^{18}O with SIII and calculated with $L = 5$ and 199 discretization points of the integral in gauge space. The two corrected curves are superimposed. Right: attempt to regularize the particle-number restored energy of ^{18}O obtained with SLy4 that contains a non-integer power of the (local) normal density.

first place and must be removed altogether. This does not only regularize spurious infinities and steps but also removes finite spurious contributions to MR energy kernels. Such a regularization method can be applied to any type of configuration mixing performed in terms of an EDF depending on *integer* powers of the density matrices. It has been successfully applied to PNR [2], as is exemplified on the left panel of Fig. 2 using the SIII Skyrme EDF together with a density-independent zero-range pairing interaction. The correction not only removes the dependence on the number of mesh points and the non-physical steps, but also corrects the energy landscape *away* from those steps. Note that the fact that the energy did not diverge in the first place at critical deformation points is specific to the analytical form of the SIII functional that only depends quadratically on the density matrix of a given isospin [2].

The case of EDFs depending on non-integer powers of the density matrix has also been analyzed [3]. Although divergences can be removed using a variant of the

method proposed in Ref. [1], the complex-plane analysis demonstrates that the left-over fractional power ρ^γ with $0 < \gamma < 1$ is ill-defined as it generates cusps in the PNR energy landscape. This is demonstrated on the right panel of Fig. 2) for a calculation based on the SLy4 Skyrme EDF complemented with a density-independent zero-range pairing interaction. Generally speaking, one cannot use a functional that is multi-valued over the complex plane. This has important consequences on the present and future of EDF methods. In particular, this calls for the design of high quality EDF parameterizations that only depend on integer powers of the density matrices.

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