Particle-Number Restoration within the Energy Density Functional formalism: Nonviability of terms depending on noninteger powers of the density matrices

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We discuss the origin of pathological behaviors that have been recently identified in particle-number-restoration calculations performed within the nuclear energy density functional framework. A regularization method that removes the problematic terms from the multi-reference energy density functional and which applies (i) to any symmetry restoration- and/or generator-coordinate-method-based configuration mixing calculation and (ii) to energy density functionals depending only on integer powers of the density matrices, was proposed in [D. Lacroix, T. Duguet, M. Bender, arXiv:0809.2041] and implemented for particle-number restoration calculations in [M. Bender, T. Duguet, D. Lacroix, arXiv:0809.2045]. In the present paper, we address the viability of non-integer powers of the density matrices in the nuclear energy density functional. Our discussion builds upon the analysis already carried out in [J. Dobaczewski *et al.*, Phys. Rev. C **76**, 054315 (2007)]. First, we propose to reduce the pathological nature of terms depending on a non-integer power of the density matrices by regularizing the fraction that relates to the integer part of the exponent using the method proposed in [D. Lacroix, T. Duguet, M. Bender, arXiv:0809.2041]. Then, we discuss the spurious features brought about by the remaining fractional power. Finally, we conclude that non-integer powers of the density matrices are not viable and should be avoided in the first place when constructing nuclear energy density functionals that are eventually meant to be used in multi-reference calculations.

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I. INTRODUCTION

In their recent paper [1], Dobaczewski *et al.* have pointed out that there are two distinct pathologies that might appear in calculations aiming at restoring particle number within the nuclear Energy Density Functional (EDF) framework. Formulating a Particle Number Restored (PNR) EDF calculation through a contour integral in the complex plane over multi-reference (MR) EDF kernels, the two categories of pathologies are associated with spurious poles and branch cuts of the complex MR-EDF kernels that relate to dependencies of the latter on integer and non-integer powers of the (transition) density matrices, respectively.

The possible appearance of spurious poles was already identified in Refs. [2–4]. In Ref. [5], hereafter referred to as Paper I, we demonstrated that such a pathology is shared by any symmetry-restoration- or generator-coordinate-method (GCM)-based configuration mixing calculation performed within the EDF context, which we will call a Multi-Reference Energy Density Functional (MR-EDF) formalism from hereon. In most other cases than PNR, however, the identification of the spuriosities is much less transparent. In Paper I, we proposed a formal and practical regularization method that applies to any symmetry restoration and/or GCM-based configuration mixing calculation. In Ref. [6], hereafter referred to as Paper II, we applied the correction method to PNR calculations using a particular energy functional that depends only on integer powers of the density matrices and thus only display spurious poles.

The pathology associated with spurious branch cuts has been overlooked until recently [1] for reasons that will become clear in the following. As a remedy to it, the authors of Ref. [1] have proposed to deform the integration contour in the complex plane such that it does not cross the branch cuts. As will be discussed below, such a procedure does not allow the definition of a fully satisfactory theory; e.g. the breaking of the shift invariance remains. In addition, there is no clear method for generalizing the proposed solution to any other coordinate frequently used in MR-EDF calculations.

In the present paper, we thus address the pathology as-

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sociated with branch cuts from a different point of view than in Ref. [1]. We first make use of the correction scheme designed in Paper I to regularize the pathology associated with spurious poles. Doing so we can isolate the part that is specific to the pathology brought about by branch cuts and question whether it is possible to perform meaningful MR calculations using an EDF that depends on non-integer powers of the density matrices. In fact, the question relates to the possibility to deal with any EDF providing multi-valued MR kernels over the complex plane. It will appear that any EDF (i) providing multi-valued MR kernels over the complex plane, (ii) whose functional form is such that the pole structure cannot be extracted analytically; e.g. the family of functionals proposed by Fayans and collaborators [7, 8], is critical. Eventually, anything but low-order polynomials seems difficult, if not impossible, to handle in practical MR-EDF calculations. Indeed, even if the pole structure of a complicated EDF can be characterized, it is only for low-order polynomials that the regularization method proposed in Paper I can be applied to identify the associated spurious contribution to the physical pole at $z = 0$.

The present discussion is conducted for PNR calculations based on a EDF whose normal part takes the form of a toy Skyrme energy density functional, and whose pairing part derives from a density-dependent delta interaction (DDDI). Numerical applications are performed using the realistic SLy4 Skyrme EDF combined with a local pairing part as derived from a (density-independent) delta interaction (DI). Two situations of interest are actually considered that correspond to using an EDF (i) derived from (density-dependent) forces (ii) formulated directly at the level of the energy functional itself.

The paper is organized as follows. In Sect. II, basic elements of the single-reference EDF method are recalled and the form of the simplified energy functional considered for the discussion is given. Section III introduces PNR calculations performed within the EDF framework and describes the analytical continuation into the complex plane which is used for analysis purposes in Sect. IV.

Section IV discusses the occurrence of pathological patterns in particle-number restored energies. First, we recall the situation for EDFs depending on integer powers of the density matrices, which is the focus of Papers I and II. Then, EDFs depending on non-integer powers of the density matrices are discussed as the simplest and most practically relevant example of EDF generating multivalued PNR energy kernels over the complex plane. Still, the conclusions drawn are valid for more involved EDFs presenting such a feature. Finally, results of numerical applications are provided in Sect. V, highlighting again the differences between EDFs depending on integer powers of the density matrices and those depending on non-integer ones. Conclusions are given in Sect. VI.

II. SINGLE-REFERENCE EDF METHOD

Before we present results obtained with a realistic SLy4+DI EDF, we analyze the relevant physics with a toy functional, reduced to the bare minimum of terms necessary to convey our point.

A. Density Matrices

The implementation of the Single-Reference EDF approach relies on the use of a quasi-particle vacuum $|\Phi_\varphi\rangle$ to calculate the one-body density matrices the energy $\mathcal{E}[\rho,\kappa,\kappa^*]$ is a functional of. The index φ in $|\Phi_\varphi\rangle$ denotes the gauge angle that provides the orientation of the system in gauge space. Using the requirement that a meaningful energy functional should be invariant under gauge space rotations, the angle can be set to a convenient value, usually $\varphi = 0$.

In the canonical basis $\{\phi_\mu(\mathbf{r}) \equiv \langle \mathbf{r}|a_\mu^\dagger|0\rangle\}$ of the Bogoliubov transformation that underlies the quasi-particle vacuum $|\Phi_0\rangle$, the SR normal density matrix ρ and anomalous density matrix κ (pairing tensor) take the form

$$\rho_{\mu\nu} \equiv \frac{\langle\Phi_0|a_\nu^\dagger a_\mu|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle} = v_\mu^2\,\delta_{\mu\nu}\,, \tag{1}$$

$$\kappa_{\mu\nu} \equiv \frac{\langle\Phi_0|a_\nu a_\mu|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle} = u_\mu v_\mu\,\delta_{\nu\bar\mu}\,, \tag{2}$$

$$\kappa^*_{\mu\nu} = \frac{\langle\Phi_0|a_\mu^\dagger a_\nu^\dagger|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle} = u_\mu v_\mu\,\delta_{\nu\bar\mu}\,, \tag{3}$$

where $\{u_\mu, v_\mu\}$ are BCS-like occupation numbers such that $u_\mu^2 + v_\mu^2 = 1$, $u_\mu = u_{\bar\mu} > 0$ and $v_\mu = -v_{\bar\mu}$. The two canonical states $(\mu, \bar\mu)$ are the so-called *pair conjugated* states. Based on an appropriate quantum number, the basis can be split into a positive half ($\mu > 0$) and a negative half ($\mu < 0$). When a canonical state μ belongs to one of these halves, its conjugate state $\bar\mu$ belongs to the other half.

From the point of view of their physical content, currently used nuclear EDFs can be put under the generic form [9]

$$\mathcal{E}[\rho,\kappa,\kappa^*] = \mathcal{E}_{\rm kin}[\rho] + \mathcal{E}_{\rm norm}[\rho] + \mathcal{E}_{\rm pair}[\rho,\kappa,\kappa^*]\,, \tag{4}$$

where appear the uncorrelated kinetic energy, the normal and the pairing contributions, respectively. The contributions from Coulomb interaction and explicit quantum corrections as the center of mass correction have been omitted for the sake of using simple notations. Including them will not modify the arguments given below. From the point of view of their functional dependence on normal and anomalous density matrices, the different parts of the functional can be formally written

$$\mathcal{E}_{\rm kin}[\rho] \equiv \mathcal{E}^{\rho}\,, \tag{5}$$

$$\mathcal{E}_{\rm norm}[\rho] \equiv \mathcal{E}^{\rho\rho} + \mathcal{E}^{\rho\rho\rho^\alpha}\,, \tag{6}$$

$$\mathcal{E}_{\rm pair}[\rho,\kappa,\kappa^*] \equiv \mathcal{E}^{\kappa\kappa} + \mathcal{E}^{\kappa\kappa\rho^\gamma}\,, \tag{7}$$

where the superscripts specify the powers of the normal and anomalous density matrices that contribute to a given term. The focus of the present work is on the properties of $\mathcal{E}^{\rho\rho\rho^\alpha}$ and $\mathcal{E}^{\kappa\kappa\rho^\gamma}$ when such a nuclear EDF is used in MR calculations. Note that the Slater approximation which is usually used to tackle the exchange part of the Coulomb contribution to the normal part of the EDF is of the form $\mathcal{E}^{\rho\rho\rho^\alpha}$.

For the sake of a transparent discussion, we will perform the analysis for a toy functional limited to the minimum of ingredients necessary to make the point. For this purpose, we start from a simplified Skyrme interaction containing the so-called t_0 and t_3 terms only, which limits the local densities entering $\mathcal{E}_{\rm norm}[\rho]$ to those that do not contain spatial derivatives [9]. In addition, and because the validity of the points made together with the conclusions reached do not critically depend on it, we omit the isospin degree of freedom and consider one nucleon species only throughout the discussion. Comments on the additional complexity brought by considering neutrons and protons are added in Sect. IV E. The generalization to a complete and realistic Skyrme or Gogny EDF is then straightforward.

B. Local densities

The local matter and spin densities needed to construct $\mathcal{E}_{\rm norm}[\rho]$ are given by

$$\rho(\mathbf{r}) \equiv \sum_\mu \phi^\dagger_\mu(\mathbf{r})\,\phi_\mu(\mathbf{r})\,\rho_{\mu\mu}\,, \tag{8}$$

$$\mathbf{s}(\mathbf{r}) \equiv \sum_\mu \phi^\dagger_\mu(\mathbf{r})\,\hat{\boldsymbol{\sigma}}\,\phi_\mu(\mathbf{r})\,\rho_{\mu\mu}\,, \tag{9}$$

where $\phi_\mu(\mathbf{r})$ and $\hat{\boldsymbol{\sigma}}$ denote a canonical single-particle spinor and the vector of Pauli matrices, respectively. In addition, one needs the local kinetic density

$$\tau(\mathbf{r}) \equiv \sum_\mu \left[\nabla\phi^\dagger_\mu(\mathbf{r})\right]\cdot\left[\nabla\phi_\mu(\mathbf{r})\right]\rho_{\mu\mu}\,, \tag{10}$$

to express the kinetic energy. The three previous local densities can be put under the form

$$f(\mathbf{r}) = \sum_\mu W^f_{\mu\mu}(\mathbf{r})\,\rho_{\mu\mu}\,, \tag{11}$$

where $f \in \{\rho, \mathbf{s}, \tau\}$ and where the explicit form of $W^f_{\mu\nu}(\mathbf{r})$ can be easily extracted from Eqs. (8-10); i.e.

$$W^\rho_{\mu\nu}(\mathbf{r}) \equiv \phi^\dagger_\mu(\mathbf{r})\,\phi_\nu(\mathbf{r})\,, \tag{12}$$

$$\mathbf{W}^s_{\mu\nu}(\mathbf{r}) \equiv \phi^\dagger_\mu(\mathbf{r})\,\hat{\boldsymbol{\sigma}}\,\phi_\nu(\mathbf{r})\,, \tag{13}$$

$$W^\tau_{\mu\nu}(\mathbf{r}) \equiv \left[\nabla\phi^\dagger_\mu(\mathbf{r})\right]\cdot\left[\nabla\phi_\nu(\mathbf{r})\right]. \tag{14}$$

The densities entering the pairing part of the EDF are the local pair densities defined as

$$\tilde\rho(\mathbf{r}) \equiv 2\sum_{\mu>0} W^{\tilde\rho}_{\mu\bar\mu}(\mathbf{r})\,\kappa_{\bar\mu\mu}\,. \tag{15}$$

Finally, with the symmetries of the SR and MR EDF calculations assumed here, $W^{\tilde\rho}_{\mu\bar\mu}(\mathbf{r})$ and $W^{\bar\rho *}_{\mu\bar\mu}$ are equal and given by the spin-singlet part of the two-body wave function, defined as

$$W^{\tilde\rho}_{\mu\nu}(\mathbf{r}) = W^{\bar\rho *}_{\mu\nu}(\mathbf{r}) \equiv \sum_{\sigma=\pm1}\sigma\,\phi_\mu(\mathbf{r}\sigma)\,\phi_\nu(\mathbf{r}-\sigma) \tag{16}$$

$$= -W^{\tilde\rho}_{\nu\mu}(\mathbf{r}) = -W^{\bar\rho *}_{\nu\mu}(\mathbf{r})\,. \tag{17}$$

C. Toy energy density functional

The kinetic energy part of the EDF takes the form

$$\mathcal{E}^\rho \equiv \int d^3r \frac{\hbar^2}{2m}\tau(\mathbf{r})\,, \tag{18}$$

whereas the normal part derives from a toy Skyrme interaction characterized by[1]

$$\mathcal{E}^{\rho\rho} \equiv \int d^3r\left[A^{\rho\rho}\rho^2(\mathbf{r}) + A^{ss}\mathbf{s}^2(\mathbf{r})\right], \tag{19}$$

$$\mathcal{E}^{\rho\rho\rho^\alpha} \equiv \int d^3r\left[A^{\rho\rho\rho^\alpha}\rho^2(\mathbf{r}) + A^{ss\rho^\alpha}\mathbf{s}^2(\mathbf{r})\right]\rho^\alpha(\mathbf{r})\,. \tag{20}$$

Finally, the pairing part of the EDF is given as

$$\mathcal{E}^{\kappa\kappa} \equiv \int d^3r\, A^{\tilde\rho\tilde\rho}\,\bar\rho^*(\mathbf{r})\,\tilde\rho(\mathbf{r})\,, \tag{21}$$

$$\mathcal{E}^{\kappa\kappa\rho^\gamma} \equiv \int d^3r\, A^{\tilde\rho\tilde\rho\rho^\gamma}\,\bar\rho^*(\mathbf{r})\,\tilde\rho(\mathbf{r})\,\rho^\gamma(\mathbf{r})\,, \tag{22}$$

where the superscripts ff and fff' of the As refer to the local densities the corresponding term depends on. In addition, one can still read off those superscripts the powers of normal and anomalous density matrices that the corresponding term incorporate. Note that no hypothesis about time-reversal invariance of the system has been made. On the other hand, we limit ourselves to quasi-particle vacua $|\Phi_\varphi\rangle$ with an even number-parity quantum number and thus only discuss explicitly even-even systems.

The part of the EDF which only depends on the normal density matrix can be derived from a schematic Skyrme *force*

$$v_{sk}(\mathbf{R},\mathbf{r}_{12}) = t_0\,(1+x_0\hat P_\sigma)\,\delta(\mathbf{r}_{12}) + \frac{t_3}{6}\,(1+x_3\,\hat P_\sigma)\,\rho_0^\alpha(\mathbf{R})\,\delta(\mathbf{r}_{12})\,, \tag{23}$$

where $\mathbf{R} \equiv (\mathbf{r}_1+\mathbf{r}_2)/2$ and $\mathbf{r}_{12} \equiv \mathbf{r}_1-\mathbf{r}_2$, whereas $\hat P_\sigma \equiv \frac{1}{2}(1+\sigma_1\cdot\sigma_2)$ denotes the spin exchange operator. Computing the normal part of the EDF as the Hartree

[1] One could have considered that the terms multiplying ρ^2 and $\mathbf{s}^2$ in $\mathcal{E}^{\rho\rho\rho^\alpha}$ present different exponents.

and Fock contributions derived from such an empirical effective vertex, one obtains

$$A^{\rho\rho} = +\tfrac{1}{4}t_0(1-x_0)\,, \quad A^{\rho\rho\rho^\alpha} = +\tfrac{1}{24}t_3(1-x_3)\,, \quad (24a)$$

$$A^{ss} = -\tfrac{1}{4}\,t_0\,(1-x_0)\,, \quad A^{ss\rho^\alpha} = -\tfrac{1}{24}t_3(1-x_3)\,, \quad (24b)$$

which shows that in this case the four coupling constants entering the EDF depend on two independent parameters only. However, we will also be interested in EDFs which are not derived from a Skyrme force and for which the four coupling constants can be chosen independently. For more complete and realistic functionals, local gauge invariance imposes constraints between certain coupling constants [10].

The part of the EDF which depends on the anomalous density matrix could be derived from the same Skyrme force. As one usually focuses on the superfluidity in the spin-singlet/isospin-triplet channel, one would be led in practice to select only a part of the interaction from the outset. Furthermore, there exists strong theoretical motivations to explicitly disconnect the part of the EDF responsible for superfluidity from the part that only depends on the normal density matrix [11]. However, such a decoupling between $\mathcal{E}_{\rm norm}$ and $\mathcal{E}_{\rm pair}$ is at the origin of serious problems encountered in MR-EDF calculations [1, 5]. We will come back to that in the following. For now, one can relate the specific local pairing functional given in Eqs. (21-22) to a DDDI vertex of the form

$$v_{\rm pair}(\mathbf{R},\mathbf{r}) = \frac{\tilde{t}_0}{2}\,(1-\hat{P}_\sigma)\left[1-\eta\Big(\frac{\rho_0(\mathbf{R})}{\rho_{sat}}\Big)^\gamma\right]\,\delta(\mathbf{r})\,, \quad (25)$$

where $\rho_{sat} = 0.16$ fm^{-3}, which leads to

$$A^{\tilde{\rho}\tilde{\rho}} = \frac{1}{4}\,\tilde{t}_0\,, \qquad A^{\tilde{\rho}\tilde{\rho}\rho^\gamma} = -\frac{\eta}{4\rho_c^\gamma}\,\tilde{t}_0\,. \quad (26)$$

Independently of the starting point, a quasi-local pairing EDF must be regularized/renormalized as far as its ultraviolet divergence is concerned [12].

III. PARTICLE NUMBER RESTORATION

A. Notations

As extensively discussed in Ref. [1] and in Paper II, Particle Number Restoration (PNR) performed within the EDF framework relies on calculating the energy of the N-particle system through a MR energy functional of the form

$$\mathcal{E}^N \equiv \int_0^{2\pi} d\varphi\,\frac{e^{-i\varphi N}}{2\pi\,c_N^2}\,\mathcal{E}[0,\varphi]\,\langle\Phi_0|\Phi_\varphi\rangle\,, \quad (27)$$

where

$$c_N^2 \equiv \int_0^{2\pi} d\varphi\,\frac{e^{-iN\varphi}}{2\pi}\,\langle\Phi_0|\Phi_\varphi\rangle\,, \quad (28)$$

in such a way that $\mathcal{E}^N$ depends only *implicitly* on the (normalized) projected state

$$|\Psi^N\rangle \equiv \frac{\hat{P}^N|\Phi_0\rangle}{\langle\Phi_0|\hat{P}^N|\Phi_0\rangle} = \int_0^{2\pi} d\varphi\,\frac{e^{-i\varphi N}}{2\pi\,c_N}\,|\Phi_\varphi\rangle\,. \quad (29)$$

The gauge-space-rotated product states constituting the MR set of interest read, in their common canonical basis, as

$$|\Phi_\varphi\rangle \equiv e^{i\varphi\hat{N}}\,|\Phi_0\rangle = \prod_{\mu>0}\Big(u_\mu + v_\mu\,e^{2i\varphi}\,a_\mu^+\,a_{\bar{\mu}}^+\Big)|0\rangle\,, \quad (30)$$

where $|0\rangle$ is the particle vacuum. The above form of $|\Phi_\varphi\rangle$ is convenient to compute the overlap between a rotated state and the unrotated one

$$\langle\Phi_0|\Phi_\varphi\rangle = \prod_{\mu>0}\left(u_\mu^2 + v_\mu^2 e^{2i\varphi}\right). \quad (31)$$

In Eq. (27), $\mathcal{E}[0,\varphi]$ denotes the (set of) MR energy density functional kernel(s). It is traditionally defined by replacing the SR normal and anomalous density matrices by transition ones

$$\rho_{\mu\nu}^{0\varphi} \equiv \frac{\langle\Phi_0|a_\nu^\dagger a_\mu|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle} = \frac{v_\mu^2\,e^{2i\varphi}}{u_\mu^2+v_\mu^2\,e^{2i\varphi}}\,\delta_{\nu\mu}\,, \quad (32)$$

$$\kappa_{\mu\nu}^{0\varphi} \equiv \frac{\langle\Phi_0|a_\nu a_\mu|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle} = \frac{u_\mu v_\mu\,e^{2i\varphi}}{u_\mu^2+v_\mu^2\,e^{2i\varphi}}\,\delta_{\nu\bar{\mu}}\,, \quad (33)$$

$$\kappa_{\mu\nu}^{\varphi 0\,*} \equiv \frac{\langle\Phi_0|a_\mu^\dagger a_\nu^\dagger|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle} = \frac{u_\mu v_\mu}{u_\mu^2+v_\mu^2\,e^{2i\varphi}}\,\delta_{\nu\bar{\mu}}\,, \quad (34)$$

into the SR EDF $\mathcal{E}[\rho,\kappa,\kappa^*]$. This corresponds to defining non-diagonal energy kernels through the prescription

$$\mathcal{E}[0,\varphi] \equiv \mathcal{E}[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\,*}]\,. \quad (35)$$

As discussed in Paper I, MR-EDF calculations performed along the lines presented above fulfill basic requirements [13] but may display pathologies such as divergences and finite steps in the energy. The extent of such problems depends on the analytical form of the EDF used. In order to conduct an in-depth analysis of the potential problems, it is necessary to perform an analytical continuation of $\mathcal{E}[0,\varphi]$ to the complex plane [1, 14].

B. Continuation to the complex plane

The continuation is achieved by extending the complex number $z = e^{i\varphi}$ onto the entire complex plane in all previous formulae.[2] In that context, the PNR energy

[2] The same notation as before is used when extending the definition of SR states and energy kernels to any value of the complex variable z. Thus, we abusively replace the gauge angle φ by the complex variable z in all our expressions; i.e. SR states characterized by the gauge angle φ, $|\Phi_\varphi\rangle$ are extended into $|\Phi_z\rangle$ to denote SR states anywhere on the complex plane. In particular, the unrotated SR state, denoted as $|\Phi_0\rangle$ when using φ as a variable, is written as $|\Phi_1\rangle$ when using z as a more general variable.

defined through Eq. (27) results from integrating over over a closed contour around $z = 0$ which can be chosen as the unit circle C_1 ($|z| = R = 1$)

$$\mathcal{E}^N \equiv \oint_{C_1} \frac{dz}{2i\pi c_N^2} \frac{\mathcal{E}[z]}{z^{N+1}} \langle \Phi_1 | \Phi_z \rangle , \quad (36)$$

$$c_N^2 = \oint_{C_1} \frac{dz}{2i\pi} \frac{1}{z^{N+1}} \langle \Phi_1 | \Phi_z \rangle , \quad (37)$$

where

$$\langle \Phi_1 | \Phi_z \rangle = \prod_{\mu>0} \left(u_\mu^2 + v_\mu^2 \, z^2 \right) . \quad (38)$$

With this continuation, the transition density matrix and pairing tensor read as

$$\rho^{1z}_{\mu\nu} = \frac{v_\mu^2 \, z^2}{u_\mu^2 + v_\mu^2 \, z^2} \, \delta_{\nu\mu} , \quad (39)$$

$$\kappa^{1z}_{\mu\nu} = \frac{u_\mu v_\mu \, z^2}{u_\mu^2 + v_\mu^2 \, z^2} \, \delta_{\nu\bar{\mu}} , \quad (40)$$

$$\kappa^{z1\,*}_{\mu\nu} = \frac{u_\mu v_\mu}{u_\mu^2 + v_\mu^2 \, z^2} \, \delta_{\nu\bar{\mu}} , \quad (41)$$

and must replace the SR density matrices in Eqs. 8-15 in order to define the corresponding transition local densities. Finally, the energy kernel from Eq. (35) reads as

$$\mathcal{E}[z] \equiv \mathcal{E}[\rho^{1z}, \kappa^{1z}, \kappa^{z1\,*}] . \quad (42)$$

IV. STEPS AND DIVERGENCES

A. General considerations

The computation of $\mathcal{E}^N$ through an integration over a contour encircling the origin requires the knowledge of the (non-)analytical structure of the integrand $\mathcal{E}[z] \langle \Phi_1 | \Phi_z \rangle / z^{N+1}$ over the complex plane. First, it obviously contains a (physical) pole at $z = 0$. Since $\mathcal{E}[z]$ is a functional of the transition density matrices, (i) it is a function of z^2 and is thus even, i.e. $\mathcal{E}[z] = \mathcal{E}[-z]$, (ii) its analytical structure relates to the one of the transition densities. As displayed in Fig. 1, it is trivial to see that ρ^{1z}, κ^{1z} and $\kappa^{z1\,*}$ possess simple poles at $z = \pm z_\mu \equiv \pm i |u_\mu|/|v_\mu|$ [1]. In general, it is likely that those poles will translate into non-analytical features of $\mathcal{E}[z] \langle \Phi_1 | \Phi_z \rangle$ that have serious consequences on the PNR energy.

As explained in Paper I, it is necessary to go to configuration space to isolate the spurious contributions to the MR-EDF energy. For a given pair of vacua belonging to the MR set, the basis relevant to the analysis of the corresponding energy kernel is the canonical basis of the Bogoliubov transformation connecting the two vacua. For PNR calculations, this simply amounts to expressing the EDF kernel $\mathcal{E}[z]$ in the canonical basis of the Bogoliubov transformation defining any of the product states of

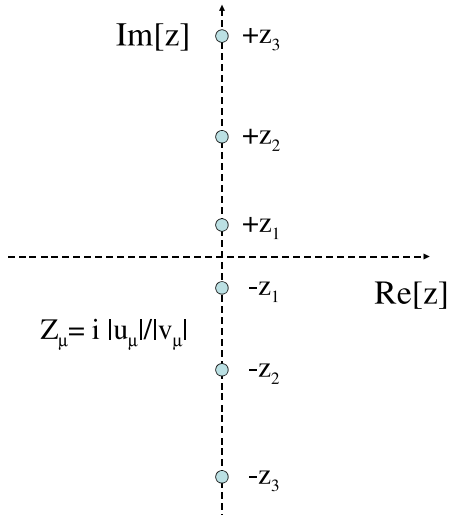

FIG. 1: Pole structure of ρ^{1z}, κ^{1z} and $\kappa^{z1\,*}$ on the complex plane.

reference; e.g. $|\Phi_1\rangle$. Indeed, the same canonical basis is shared by all product states $|\Phi_z\rangle$ over the complex plane, as well as by the Bogoliubov transformation linking any pair of them.

B. Term depending on integer powers of densities

Let us start the analysis with terms that depend on integer powers of the density matrices. To illustrate the situation, we make use of the bilinear parts, Eqs. (19) and (21), of the toy EDF introduced in Sect. II C.

1. Matrix elements

Working in the canonical basis of Bogoliubov transformation connecting $|\Phi_1\rangle$ and $|\Phi_z\rangle$, the bilinear part of the energy kernel $\mathcal{E}[z]$ takes the form

$$\mathcal{E}^{\rho\rho}[z] + \mathcal{E}^{\kappa\kappa}[z] = \tfrac{1}{2} \sum_{\mu\nu} \bar{v}^{\rho\rho}_{\mu\nu\mu\nu} \, \rho^{1z}_{\mu\mu} \, \rho^{1z}_{\nu\nu} + \tfrac{1}{4} \sum_{\mu\nu} \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\nu\bar{\nu}} \, \kappa^{z1\,*}_{\mu\bar{\mu}} \, \kappa^{1z}_{\nu\bar{\nu}} , \quad (43)$$

where $\bar{v}^{\rho\rho}$ and $\bar{v}^{\kappa\kappa}$ denote matrix elements of *effective* two-body vertices associated with $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$, respectively. For the toy functional of Eq. (19), the matrix elements of $\bar{v}^{\rho\rho}$ take the form

$$\bar{v}^{\rho\rho}_{\mu\nu\mu\nu} \;\equiv\; 2\int d^3r\,\left[A^{\rho\rho}\,W^{\rho}_{\mu\mu}(\mathbf{r})\,W^{\rho}_{\nu\nu}(\mathbf{r}) + A^{ss}\,\mathbf{W}^{s}_{\mu\mu}(\mathbf{r})\cdot\mathbf{W}^{s}_{\nu\nu}(\mathbf{r})\right]\,. \tag{44}$$

The quasi-local nature of the Skyrme energy functional (the toy functional considered here being purely local) simplifies the construction of the matrix elements $\bar{v}^{\rho\rho}_{\mu\nu\mu\nu}$ as they involve a single spatial integral only. However, the discussion conducted in the rest of the paper would hold equally for non-local functionals; e.g. as obtained from finite-range, possibly non-local, effective vertices.

The matrix elements associated with $\mathcal{E}^{\kappa\kappa}$ in Eq. (21) take the form

$$\bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\nu\bar{\nu}} \equiv 4\int d^3r\;A^{\tilde{\rho}\tilde{\rho}}\,W^{\bar{\mu}*}_{\mu\bar{\mu}}(\mathbf{r})\,W^{\tilde{\rho}}_{\nu\bar{\nu}}(\mathbf{r})\;. \tag{45}$$

Note that for PNR calculations, the matrix elements that one naturally associate to any term of the EDF depending on integer powers of the density matrices do not depend on the pair of vacua $|\Phi_1\rangle$ and $|\Phi_z\rangle$ under consideration, i.e. they do not depend on the gauge variable z.

2. *Analytical structure of* $(\mathcal{E}^{\rho\rho}[z] + \mathcal{E}^{\kappa\kappa}[z])\,\langle\Phi_1|\Phi_z\rangle$

Due to the additional presence of the norm factor $\langle\Phi_1|\Phi_z\rangle$ in the integrand of Eq. (36), it is easy to realize that only the terms corresponding to $\nu=\mu$ and $\nu=\bar{\mu}$ in Eq. (43) can lead to non-analytical features [5, 6]. Such terms contribute to the integrand through

$$\nu=\mu \implies \tfrac{1}{2}\left(\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}+\bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}}\right)\frac{v_\mu^4\,z^4}{u_\mu^2+v_\mu^2\,z^2}\prod_{\nu\neq\mu>0}\left(u_\nu^2+v_\nu^2\,z^2\right)\,, \tag{46}$$

$$\nu=\bar{\mu} \implies \left[\tfrac{1}{2}\left(\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}}+\bar{v}^{\rho\rho}_{\bar{\mu}\mu\bar{\mu}\mu}\right)v_\mu^2\,z^2+\bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}\,u_\mu^2\right]\frac{v_\mu^2\,z^2}{u_\mu^2+v_\mu^2\,z^2}\prod_{\nu\neq\mu>0}\left(u_\nu^2+v_\nu^2\,z^2\right)\,, \tag{47}$$

and both contain potential poles at $z=\pm z_\mu=\pm i|u_\mu|/|v_\mu|$. Note that those poles do not exist in the first place if the states $(\mu,\bar{\mu})$ are more than doubly degenerate in terms of occupation numbers as an additional factor from the norm then compensates the single pole in Eqs. (46-47).[3]

Otherwise, the poles disappear in Eq. (46) if, and only if, $\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}=\bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}}=0$; i.e. the matrix elements associated with $\mathcal{E}^{\rho\rho}$ are antisymmetrized. Coming back to the toy Skyrme functional used in the present paper, and noticing that

$$|\mathbf{W}^{s}_{\mu\mu}(\mathbf{r})|^2 = |W^{\rho}_{\mu\mu}(\mathbf{r})|^2 = \Big[\sum_{\sigma=\pm1}|\varphi_\mu(\mathbf{r}\sigma)|^2\Big]^2\,, \tag{48}$$

for all μ, one finds that $\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}=\bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}}=0$ if, and only if, $A^{ss}=-A^{\rho\rho}$. As shown by Eqs. (24a-24b), such a condition is satisfied when starting from the (density-independent part of the) Skyrme *force*. The previous analysis is trivially extended to the density-independent part of a more complete Skyrme or Gogny vertex. On the other hand, using a functional approach that bypasses the introduction of a two-body vertex, relationships such as $A^{ss}=-A^{\rho\rho}$ might not be fulfilled. In such a case $\mathcal{E}^{\rho\rho}$ generates poles at $z=\pm z_\mu$ in the integrand of Eq. (36).

The poles disappear from Eq. (47) if, and only if, $\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}}=\bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}$; i.e. diagonal matrix elements involving two conjugated canonical states are identical in $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$. If it is so, the two terms in the bracket of Eq. (47) combine in such a way that the dangerous denominator explicitly cancels out. One is then left with a finite contribution to the MR energy kernel. Such a recombination is obviously satisfied if both $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$ are constructed from the same (effective) force, for example when using the density-independent part of the Gogny interaction [3]. Using a functional approach or starting from two different effective vertices to build $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$, the recombination is unlikely to occur and one is left with an ill-defined PNR formalism and compromised results. Just as we did to ensure that $\bar{v}^{\rho\rho}_{\mu\mu\mu\mu}=\bar{v}^{\rho\rho}_{\bar{\mu}\bar{\mu}\bar{\mu}\bar{\mu}}=0$, i.e. $A^{ss}=-A^{\rho\rho}$, one could work out minimal constraints between the coupling constants entering $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$ to

[3] This holds for bilinear functionals. A term of order n in the density matrices can generate a pole at $\pm z_\mu$ of order (at most) $(n-1)$. For the pole to disappear, $(n-1)$ additional factors from the norm kernel are needed to cancel the denominator $(u_\mu^2+v_\mu^2\,z^2)^{-(n-1)}$. Thus, the pair of interest $(\mu,\bar{\mu})$ needs to be degenerate (at least) with $(n-1)$ other pairs in terms of occupations for this to occur.

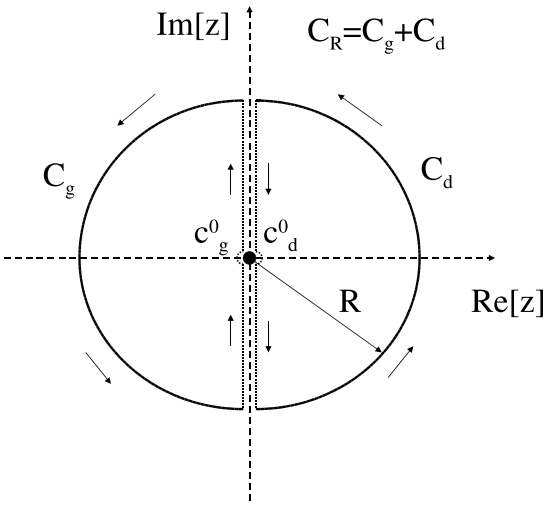

FIG. 2: Computation of $\mathcal{E}^N$ for an EDF (i) obtained from the average value of a genuine Hamiltonian in the projected state (ii) depending only on integer powers of the densities and after applying the correction proposed in Paper I. The integration is performed in the complex plane over a circular contour C_R of arbitrary radius R.

impose that $\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} = \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}$ in the underlying EDF.

3. Projected energy from a Hamiltonian

As seen from the previous discussion, poles in the transition densities do not always translate into poles in $\mathcal{E}[z]\,\langle\Phi_1|\Phi_z\rangle$. The most trivial example for this occurs when the particle number projected energy is computed from the average value of a genuine Hamiltonian in the projected state $|\Psi^N\rangle$; i.e. what we denote as the strict projected HFB approach in Paper II. In this case, the only pole of the integrand in Eq. (36) is the physical one at $z = 0$. To apply the Cauchy theorem[4] and calculate the projected energy, the original circular contour $\mathcal{C}_1$ must be deformed to exclude the pole at $z = 0$. As shown in Fig. 2, this can be achieved by choosing two semi-circular contours C_d and C_g, such that $C_1 \equiv \big[C_g + C_d\big](\epsilon \to 0)$, and by closing those semi-circular contours along the imaginary axis in such a way that the pole at $z = 0$ is bypassed by two semi-circles of infinitely small radii. Using such contours, it is easy to prove that

$$c_N^2\,\mathcal{E}^N \;=\; \mathcal{R}es\left[\frac{\mathcal{E}[z]\,\langle\Phi_1|\Phi_z\rangle}{z^{N+1}}\right]\Bigg|_{z=0}, \qquad (49)$$

$$c_N^2 \;=\; \mathcal{R}es\left[\frac{\langle\Phi_1|\Phi_z\rangle}{z^{N+1}}\right]\Bigg|_{z=0}. \qquad (50)$$

Because the only pole of the integrand is at $z = 0$, the same result is obtained for $\mathcal{E}^N$ by starting from any integration contour encircling the origin in Eq. (36). When the energy is calculated as the average value of a Hamiltonian in the projected state, the independence of the projected energy on the details of the integration contour, as for example its radius, can be related to the invariance of the normalized projected state with respect to *shift transformations* [1, 14]. This symmetry will be discussed below in the EDF context.

4. PNR energy from an EDF

The poles subsist in Eqs. (46) and (47) for any EDF that is characterized by $\bar{v}^{\rho\rho}_{\mu\mu\mu\mu} \neq 0$ and/or $\bar{v}^{\rho\rho}_{\mu\bar{\mu}\mu\bar{\mu}} \neq \bar{v}^{\kappa\kappa}_{\mu\bar{\mu}\mu\bar{\mu}}$. To apply the Cauchy theorem in this case, the circular contour C_1 must now be deformed to exclude not only the pole at $z = 0$ but also those at $z = \pm z_\mu$ which are inside the unit circle. As shown in Fig. 3, this can be done by choosing two semi-circular contours C_d and C_g, such that $C_1 \equiv \big[C_g + C_d\big](\epsilon \to 0)$, and by closing each of them along the imaginary axis in such a way that all the poles are bypassed by semi-circles of infinitely small radii. Using such contours, the Cauchy theorem leads to

$$c_N^2\,\mathcal{E}^N \;=\; \sum_{z=0,\pm z_\mu} \mathcal{R}es\left[\frac{\mathcal{E}[z]\,\langle\Phi_1|\Phi_z\rangle}{z^{N+1}}\right]\Bigg|_{z}, \qquad (51)$$

whereas c_N^2 remains unchanged.

According to Eq. (51), the existence of poles at $z = \pm z_\mu$ in the integrand makes the PNR energy to (i) depend on the radius of the integration circle [1, 6] (ii) display a finite step whenever a pole leaves the integration circle; e.g. as the system is deformed along a collective degree of freedom [1, 6]. Such a behavior make the PNR energy to break shift invariance. This is very undesirable as the concept of shift transformation and shift invariance can be extended to the EDF framework in such a way that the invariance of $\mathcal{E}^N$ with respect to the radius of the integration contour remains a fundamental feature of the theory [15].

Also, PNR energies may display divergences whenever a pole crosses the integration circle. When a pole sits on the integration contour C_R, the definition of the contour $C_R \equiv \big[C_g + C_d\big](\epsilon \to 0)$ is in fact ambiguous and requires an additional prescription. The most natural procedure is to define the integration through the pole in the sense of the Cauchy principal value. Doing so provides a finite PNR energy if the Laurent series of the integrand centered at the pole only contains odd powers. Considering

[4] The present Section reformulates parts of the analysis proposed in Paper II for functionals proportional to integer powers of the density matrices, i.e. we employ Cauchy's integral theorem rather than using directly Cauchy's residue formula. Coming back to Cauchy's integral theorem will be needed to conduct the discussion for more general functionals as is indicated in the next Section.

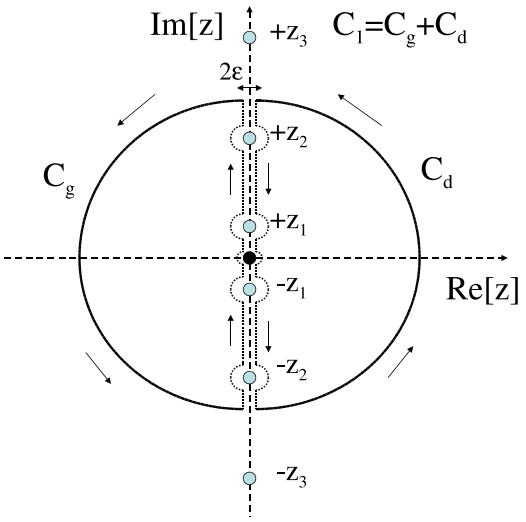

FIG. 3: Computation of $\mathcal{E}^N$ for an EDF depending on integer powers of the densities. The integration is performed in the complex plane over the unit circle C_1.

the structure of the nuclear EDF, this will happen if the EDF (i) only contains bilinear terms (ii) contains additional trilinear terms that do not allow three powers of the same isospin (as a zero-range three-body force does not allow) (iii) contains additional quartic terms which are bilinear in each isospin. In this case, one is left with simple poles at $z = \pm z_\mu$ and the Cauchy principal value equals half the result that would be obtained if the pole were to lie inside the integration circle. In all other cases, one can see that (i) the poles at $z = \pm z_\mu$ will be of higher orders (ii) the Laurent series centered at those poles will contain even powers (ii) the Cauchy principle value will lead to an infinite values and the PNR energy will diverge as a poles crosses the integration circle. If the EDF used is such that PNR energies diverge whenever a pole crosses the integration circle, it is important to note that Variation After Projection (VAP) calculations will not converge as soon as the minimization procedure "finds" the infinity [3, 16].

All previous features prove that PNR calculations are ill-defined whenever poles at $z \neq 0$ arise and that the theory is unacceptable as it is. However, it is possible to meaningfully regularize PNR calculations based on any EDF depending on integer powers of the density matrices as was demonstrated in Paper I and exemplified in Paper II. As a matter of fact, the method proposed in Paper I precisely removes the poles at $z = \pm z_\mu$ from $\mathcal{E}[z]\,\langle\Phi_1|\Phi_z\rangle$. However, it is crucial to realize that the correction method does not only remove those poles but also consistently subtracts a spurious contribution to the physical pole at $z = 0$ [6]. In the end, only the physical pole at $z = 0$ remains in Eq. (49) and the independence of $\mathcal{E}^N$ on the integration contour is recovered, as seen from Fig. 2; i.e. the same PNR energy is obtained by integrating over circular contours C_R of arbitrary radius R.

C. Non-integer power of densities

1. Problem

The situation is often more complex due to the presence of higher-order terms of the form $\mathcal{E}^{\rho\rho\rho^\alpha}$ and $\mathcal{E}^{\kappa\kappa\rho^\gamma}$ in realistic nuclear EDFs, Eqs. (20) and (22).

If $\alpha = \gamma = 1$, then $\mathcal{E}^{\rho\rho\rho}$ and $\mathcal{E}^{\kappa\kappa\rho}$ can, at least formally, be analyzed as if they originated from a three-body vertex. Thus, and as for the bilinear terms, two cases have to be distinguished (i) $\mathcal{E}^{\rho\rho\rho}$ and $\mathcal{E}^{\kappa\kappa\rho}$ are both derived from the same antisymmetrized three-body vertex and do not lead to divergences and steps in MR-EDF calculations (ii) they refer to different three-body vertices such that the regularization method proposed in Paper I can be applied to obtain a meaningful PNR-EDF method.

However, all modern parameterizations of the nuclear EDF, starting either from a functional approach or from a density-dependent vertex, depend on non-integer powers of the density matrix that one cannot expand in a Taylor series to relate them, at least formally, to three-body, four-body, ... forces. The goal of the present paper is to characterize the pathologies brought about by such dependencies and whether or not they are viable in the end; i.e. if the corresponding pathologies can be easily regularized.

2. Regularizing the integer part

As a first step, one can reduce the extent of the problems associated with terms of the form $\mathcal{E}^{\rho^{2m+n+\alpha}}$ and $\mathcal{E}^{\kappa^{2m}\rho^{n+\gamma}}$, with m and n integer, and $0 < \alpha < 1$ and $0 < \gamma < 1$, to pathologies only due to the fractional powers ρ^α and ρ^γ, respectively. This means that steps and potential divergences associated with the *integer part* $2m + n$ can be regularized from the outset. This is the case either (i) if one started from a density-dependent $(2m + n)$-body effective force or (ii) by applying the correction method proposed in Paper I to $\mathcal{E}^{\rho^{2m+n}}$ and $\mathcal{E}^{\kappa^{2m}\rho^n}$.

Let us exemplify how an empirical extension of the correction method proposed in Paper I can be designed to regularize the quadratic part of $\mathcal{E}^{\rho\rho\rho^\alpha}$, with $0 < \alpha < 1$. To simplify the situation further, we disregard the term $\mathcal{E}^{\kappa\kappa\rho^\gamma}$ in the following discussion. Such a simplification does not alter any of the conclusions given in the rest of the paper.

To proceed, we first introduce *pseudo* two-body matrix elements $\bar{v}^{\rho\rho\rho^\alpha}_{\mu\nu\mu\nu}[z]$ which take, for the toy functional considered in the present paper, the form

$$\bar{v}^{\rho\rho\rho^\alpha}_{\mu\nu\mu\nu}[z] \;\equiv\; 2\int d^3r\,\left[A^{\rho\rho\rho^\alpha}\,W^{\rho}_{\mu\mu}(\mathbf{r})\,W^{\rho}_{\nu\nu}(\mathbf{r}) + A^{ss\rho^\alpha}\,\mathbf{W}^{s}_{\mu\mu}(\mathbf{r})\cdot\mathbf{W}^{s}_{\nu\nu}(\mathbf{r})\right]\left[\rho^{1z}(\mathbf{r})\right]^\alpha . \tag{52}$$

With the pseudo two-body matrix elements $\bar{v}^{\rho\rho\rho^\alpha}_{\mu\nu\mu\nu}[z]$ at hand, one can apply the correction formula given by Eq. (43) of Paper II. However, and as opposed to terms of the EDF depending on integer powers of the density matrices, the matrix elements of $\bar{v}^{\rho\rho\rho^\alpha}$ do depend on the gauge variable z. As a result, Eq. (43) of Paper II must be applied in such a way that the matrix elements are located underneath the integral over z. Last but not least, it would also be trivial to regularize the integer part of $\mathcal{E}^{\kappa\kappa\rho^\gamma}$ by introducing the pseudo two-body matrix elements $\bar{v}^{\kappa\kappa\rho^\alpha}[z]$ and by using them in Eq. (43) of Paper II.

D. Left-over fractional power

With the latter correction at hand, the quadratic part of $\mathcal{E}^{\rho\rho\rho^\alpha}$ does not create any divergence or step in the PNR-EDF energy anymore. Again, the same is true if one starts from the outset from a density-dependent two-body antisymmetrized *interaction*, as long as the corresponding term $\mathcal{E}^{\kappa\kappa\rho^\alpha}$ is explicitly considered in the EDF to proceed to the necessary recombination of terms in Eq. (47). One way or another, one is only left in the end with discussing the impact of the *fractional* power of the transition density; i.e. the extra factor $\left[\rho^{1z}(\mathbf{r})\right]^\alpha$, with $0<\alpha<1$.

1. *Analytical structure of* $\mathcal{E}^{\rho\rho\rho^\alpha}[z]\,\langle\Phi_1|\Phi_z\rangle$

Now that the pathologies due to the bilinear factor in $\mathcal{E}^{\rho\rho\rho^\alpha}$ have been taken care of, the contribution of interest to the PNR energy can be written as

$$\mathcal{E}^N[\rho\rho\rho^\alpha] \equiv \oint_{C_R}\frac{dz}{2i\pi c_N^2}\,\frac{\mathcal{E}^{\rho\rho\rho^\alpha}[z]}{z^{N+1}}\,\langle\Phi_1|\Phi_z\rangle \equiv \oint_{C_R}\frac{dz}{2i\pi c_N^2}\int d^3r\,\frac{F[z](\mathbf{r})}{z^{N+1}}\left[\rho^{1z}(\mathbf{r})\right]^\alpha , \tag{53}$$

where

$$F[z](\mathbf{r}) \;\equiv\; z^4\sum_{\nu\neq\mu,\bar{\mu}}\left[A^{\rho\rho\rho^\alpha}\,W^{\rho}_{\mu\mu}(\mathbf{r})\,W^{\rho}_{\nu\nu}(\mathbf{r}) + A^{ss\rho^\alpha}\,\mathbf{W}^{s}_{\mu\mu}(\mathbf{r})\cdot\mathbf{W}^{s}_{\nu\nu}(\mathbf{r})\right] v_\mu^2\,v_\nu^2\prod_{\substack{\zeta>0\\ \zeta\neq\mu,\nu}}\left(u_\zeta^2+v_\zeta^2\,z^2\right), \tag{54}$$

with N even. In agreement with the properties of $\mathcal{E}[z]$ mentioned above, $F[z](\mathbf{r})$ is an even function of z for all $\mathbf{r}$. For odd N, it is easy to prove that $F[z](\mathbf{r})$ is an odd function of z in such a way that $F[z](\mathbf{r})/z^{N+1}$ remains itself an odd function of z.

The terms corresponding to $\nu=\mu$ and $\nu=\bar{\mu}$ are absent in Eq. (54) because (i) they were removed by the correction method briefly outlined in Sect. IV C (ii) one started from a density-dependent two-body interaction; i.e. the term with $\nu=\mu$ do disappear ($A^{ss\rho^\alpha}=-A^{\rho\rho\rho^\alpha}$) whereas the term with $\nu=\bar{\mu}$ could be combined with the corresponding one in $\mathcal{E}^{\kappa\kappa\rho^\alpha}$ to give a well-behaved contribution that we omit here.

To understand the features displayed by the contribution $\mathcal{E}^N[\rho\rho\rho^\alpha]$ to the PNR energy, it is necessary to extract for each $\mathbf{r}$ the non-analytical structure of the integrand in Eq. (53) where the order of the two integrals over $\mathbf{r}$ and z have been reversed. Clearly, the function $F[z](\mathbf{r})/z^{N+1}$ displays a (physical) pole at $z=0$. The difficulty comes from the fractional power of the local transition density that multiplies $F[z](\mathbf{r})$. Indeed, such a function is multivalued on the complex plane for all $\mathbf{r}$.

Defining the function corresponding to taking the fractional power of a complex number[5] requires the introduction of a branch cut along the axis where that number is real and negative. Here, this means that one needs the values of z for which the function $\rho^{1z}(\mathbf{r})$ is real and negative. As can be seen from Eqs. (8) and (39), the transition density is real both on the real and imaginary axis, but can be negative only on the latter. A discussed in Ref. [1], $\rho^{1z}(\mathbf{r})$ is negative for $z=iy$ such

[5] Parameterizing $z=re^{i\theta}$, $\theta\in[-\pi,+\pi]$, we define the principal value of the function z^α, α being a rational number between zero and one, as $z^\alpha\equiv r^\alpha e^{i\alpha\theta}$. The latter choice lifts the ambiguity regarding the multivalued nature of the function but requires to track the latter through several Riemann cuts.

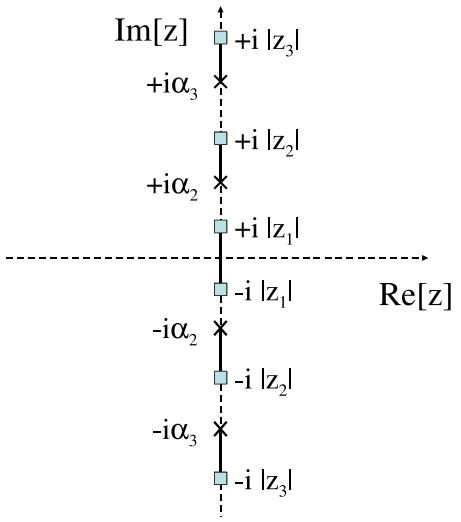

FIG. 4: Branch cuts of $\left[\rho^{1z}(\mathbf{r})\right]^{\alpha}$. The branch cuts join the integrable poles of $\left[\rho^{1z}(\mathbf{r})\right]^{\alpha}$ at $z = \pm i|u_\mu/v_\mu|$ (squares) and its zeros at $z = \pm i\alpha_\mu$ (crosses).

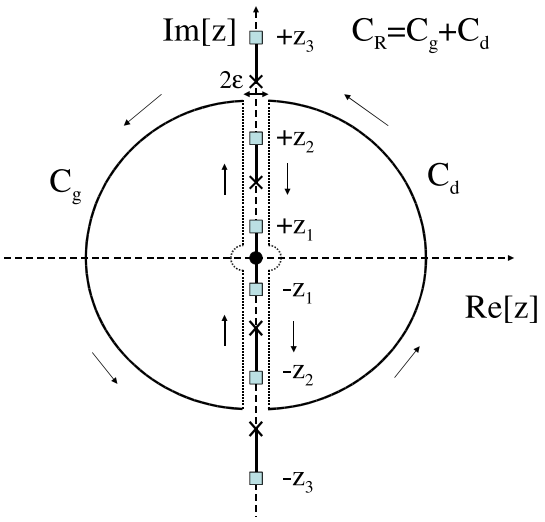

FIG. 5: Specification of the integration contour for an EDF containing fractional powers of the densities.

that $|z_{\mu-1}| < \alpha_\mu < y < |z_\mu|$, as well as on the entire interval $[-z_1, +z_1]$, where z_1 denotes the closest pole to the origin. The corresponding branch cuts are characterized in Fig. 4 by solid lines joining the zeros of $\rho^{1z}(\mathbf{r})$ at $z = \pm i\alpha_\mu$ (crosses) and its next integrable pole at $z = \pm z_\mu$ (square). Whereas the poles of $\rho^{1z}(\mathbf{r})$ are independent of the position vector $\mathbf{r}$, the points $z = \pm i\alpha_\mu$ at which it changes sign in between two poles do depend on $\mathbf{r}$.

2. *Calculation of* $\mathcal{E}^N[\rho\rho\rho^\alpha]$

Knowing the non-analytical structure of the integrand $F[z](\mathbf{r})\left[\rho^{1z}(\mathbf{r})\right]^{\alpha}/z^{N+1}$, the integration contour to be used in Eq. (53) can be specified. Just as before, the circle C_R needs to be deformed in order to apply the Cauchy theorem on contours encircling regions where the function is entirely analytical. In particular, one cannot go through branch cuts as one must remain on the same Riemann sheet. An acceptable decomposition under the form $C_R \equiv \left[C_g + C_d\right](\epsilon \to 0)$, where each semi-circle C_g/C_d is further closed by a vertical segment along the imaginary axis interrupted by a semi-circle around the origin, is displayed in Fig. 5. Note that, as opposed to Fig. 3, no special care needs to be taken around the poles at $z = \pm z_\mu$ as they are now integrable ($\sim 1/z^\alpha$ with $0 < \alpha < 1$). The crucial point, however, is that the portions along the branch cuts will not cancel out as we sum the two vertical segments because the integrand (in fact $\left[\rho^{1z}(\mathbf{r})\right]^{\alpha}$) is discontinuous across the branch cuts.

One may wonder what happens when, as in Fig 6, the radius R is such that the original contour C_R goes through a branch cut. In fact, the contour C_R defined through $\left[C_g + C_d\right](\epsilon \to 0)$ in Fig. 5 (i) is well defined when a branch cut lies in between C_g and C_d because the limit $\epsilon \to 0$ does not pose any problem once the value of the function on both sides of the cut has been properly worked out, (ii) is the contour which has been used in actual calculations [1, 3, 17] and (iii) might however need to be discretized on a rather dense mesh to provide converged calculations.

Note that the deformation of the contour discussed above was advocated in Ref. [1] as a remedy to the pathology brought about by branch cuts. In fact, it is rather a necessary step to simply *define* the integration over the original circle and obtain the result it provides. As detailed below, proceeding to such a deformation of the contour does not remove the intrinsic pathological nature of MR calculations performed using an EDF containing non-integer powers of the density matrices.

We are now ready to apply the Cauchy theorem along the two closed contours appearing in Fig. 5 and then let ε goes to zero. It is clear that the contributions from the vertical portions in between the branch cuts cancel out as we add the results from the two closed contours. On the other hand, contributions from segments along the branch cuts will not cancel out because of the discontinuity of the integrand across them.

We consider for illustration (see Fig. 6) the situation where the contour C_R "hits" the $(n+1)^{th}$ branch cut at $z = \pm iR$; i.e. $\alpha_{n+1} \leq R \leq |z_{n+1}|$. This means that the n^{th} branch cut is entirely located inside C_R whereas the $(n+1)^{th}$ one is partially outside the circle of integration. For simplicity, and because it is irrelevant to the present discussion, we do not calculate the contribution $\mathcal{E}^N[\rho\rho\rho^\alpha]([-z_1, +z_1])$ from the closest branch cut to the origin. Indeed, this one is trickier than the other branch cuts because the physical pole at $z = 0$ lies on that branch

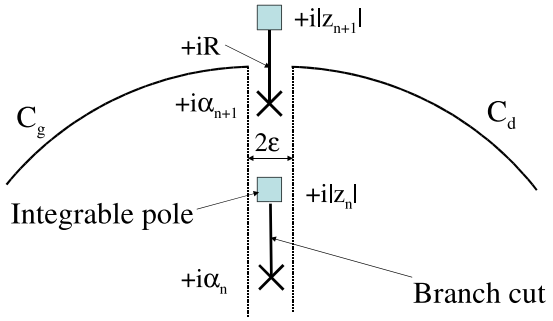

FIG. 6: Zoom on the integration contour $\mathcal{C}_R$ obtained as the limit of the sum of two disconnected semi-circles. For illustration, we display a situation where the chosen integration contour C_R "hits" the $(n+1)^{th}$ branch cut at $z = \pm iR$, that is, has a radius R such that $\alpha_{n+1} \leq R \leq |z_{n+1}|$.

cut. All that matters for the present discussion is that the branch cut $[-z_1, +z_1]$ provides a finite contribution to the projected energy. In the end, one obtains

$$\mathcal{E}^N[\rho\rho\rho^\alpha](R) - \mathcal{E}^N[\rho\rho\rho^\alpha]([-z_1,+z_1]) \;=\; (-1)^{\frac{N}{2}}\,\frac{2}{\pi}\,\sin(\alpha\pi)\left[\sum_{\mu=1}^{n}\int_{\alpha_\mu}^{|z_\mu|}dy + \int_{\alpha_{n+1}}^{R}dy\right]\int d^3r\,\frac{F[iy](\mathbf{r})}{y^{N+1}}\left|\rho^{1\,iy}(\mathbf{r})\right|^\alpha \quad (55)$$

which is real and where, for y real,

$$\rho^{1\,iy}(\mathbf{r}) \;=\; \sum_\mu W^\rho_{\mu\mu}(\mathbf{r})\,\frac{y^2}{y^2-|z_\mu|^2}\,, \quad (56)$$

$$F[iy](\mathbf{r}) \;=\; y^4\sum_{\nu\neq\mu,\bar\mu}\left[A^{\rho\rho\rho^\alpha}\,W^\rho_{\mu\mu}(\mathbf{r})\,W^\rho_{\nu\nu}(\mathbf{r}) + A^{ss\rho^\alpha}\,\mathbf{W}^s_{\mu\mu}(\mathbf{r})\cdot\mathbf{W}^s_{\nu\nu}(\mathbf{r})\right]v_\mu^2\,v_\nu^2\prod_{\substack{\zeta>0\\ \zeta\neq\mu,\nu}}(u_\zeta^2 - v_\zeta^2\,y^2)\,. \quad (57)$$

The above analytical results are explicit enough that we can draw several important conclusions from them. First, Eq. (55) demonstrates that the PNR energy depends on the radius R of the integration contour through the boundary of the integral; i.e. the PNR energy is not shift invariant. As C_R goes through a branch cut, the contribution of that branch cut changes progressively and leaves a smoothed step in the PNR energy; see Fig. 7. This relates to an unphysical breaking of shift invariance. Second, there is no discontinuity or divergence as C_R passes through the branch points since the function $|\rho^{1\,iy}(\mathbf{r})|^\alpha$ is integrable at $y = |z_\mu|$, for all μ.

The two previous conclusions are at variance with what happens for (most of the) EDFs containing only integer powers of the densities as recalled in Sect. IV B. Indeed, a pole crossing the integration provides in this case PNR energies with (i) an abrupt step (ii) a divergence if the pole is of even order [6]. Also, it is important to underline the role played by the regularization of the bilinear part of $\mathcal{E}^{\rho\rho\rho^\alpha}$ put forward in Sect. IV C 2. If one were to use the *uncorrected* term $\mathcal{E}^{\rho\rho\rho^\alpha}$, the PNR energy would diverge as C_R passes through the branch points. Indeed, the integrand in Eq. (55) would then contain terms overall proportional to $(y^2 - |z_\mu|^2)^{-1}|\rho^{1\,iy}(\mathbf{r})|^\alpha$ which is *not* integrable at $y = |z_\mu|$.

In any case, the absence of divergence for the *regularized* $\mathcal{E}^N[\rho\rho\rho^\alpha]$ is critical since the associated integrability of the pole was used in Ref. [3] to assess the meaningfulness of PNR calculations performed with the Gogny force. However, and although divergences do constitute a dramatic pathology of ill-defined PNR calculations, the most profound problem relates rather to the breaking of shift invariance of the PNR energy as one changes the integration contour. Indeed, the associated spurious branch cuts modify the topology of potential energy curves as one deforms the system with respect to a col-

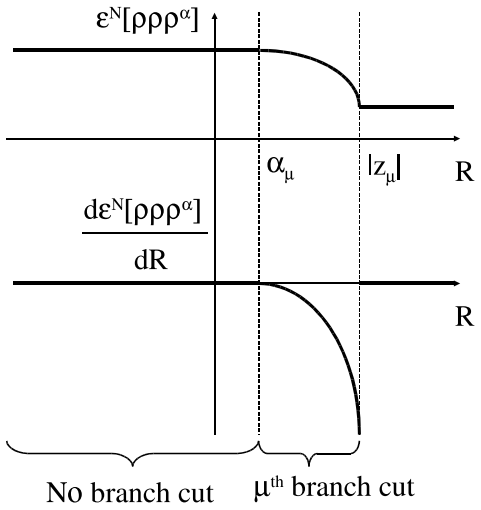

FIG. 7: Schematic effect of a shift transformation on the PNR energy. Top: projected energy $\mathcal{E}^N[\rho\rho\rho^\alpha]$ as a function of R. Bottom: same for the derivative of $\mathcal{E}^N[\rho\rho\rho^\alpha]$ with respect to R.

lective degree of freedom. As discussed above, such a problem persists for a regularized non-integer power or, equivalently, for an effective two-body vertex depending on a fractional power of the density. Still, the absence of divergence explains why the spurious nature of fractional powers of the densities that we focus on here has been overlooked so far even more than the pathologies brought about by integer powers.

In the end, divergences are presently replaced by another pathological behavior of the PNR energy. To isolate such a pattern, let us take the derivative of $\mathcal{E}^N[\rho\rho\rho^\alpha](R)$ in Eq. (55) with respect to the radius of integration R. One obtains, for $\mu > 1$

$$\left.\frac{d\mathcal{E}^N[\rho\rho\rho^\alpha]}{dR}\right|_R = \begin{cases} 0 & \text{if } R \in \left[|z_{\mu-1}|, \alpha_\mu\right] , \\ \dfrac{(-1)^{N/2}}{R^{N+1}}\,\dfrac{2}{\pi}\,\sin(\alpha\pi)\int d^3r\; F[iR](\mathbf{r})\left|\rho^{1\,iR}(\mathbf{r})\right|^\alpha & \text{if } R \in \left[\alpha_\mu, |z_\mu|\right]. \end{cases} \tag{58}$$

Because of the non-analytic behavior of $\left|\rho^{1\,iR}(\mathbf{r})\right|^\alpha$ at each branch point, the derivative diverges in Eq. (58) for $R = |z_\mu|$, $\mu \neq 1$. As a result, the projected energy displays a *kink* (non-derivable behavior) as the integration circle goes through a branch point or as a branch point goes through the integration circle when the system is deformed along a collective path. This fact alone is unacceptable for a well-defined projected theory. The corresponding pattern is schematically displayed in Fig. 7 and is observed in realistic calculations as will be discussed in Sect. V.

E. Isospin degree of freedom

The isospin degree of freedom does not modify any conclusion of the present paper but only complexifies certain aspects of the discussion. Still, to provide an idea of the modifications brought about by the consideration of both protons and neutrons, we now proceed to a restricted set of remarks.

Considering the isospin degree of freedom, one must account for the fact that densities, e.g. $\rho_q(\mathbf{r})$, and single-particle wave-functions $\varphi_\mu(\mathbf{r}q)$ are now labeled with the isospin projection quantum number q, where $q = n$ and $q = p$ for neutrons and protons, respectively. The problematic terms entering the toy Skyrme functional (Eqs. 20-22) now take the form

$$\begin{aligned} \mathcal{E}^{\rho\rho\rho^\alpha} \;\equiv\; & \int d^3r \sum_{q=p,n} \left[A^{\rho\rho\rho^\alpha}\,\rho_q^2(\mathbf{r}) + A^{ss\rho^\alpha}\,\mathbf{s}_q^2(\mathbf{r})\right]\rho_0^\alpha(\mathbf{r}) \\ & + \int d^3r \sum_{\substack{q,q'=p,n \\ q\neq q'}} \Big[B^{\rho\rho\rho^\alpha}\,\rho_q(\mathbf{r})\,\rho_{q'}(\mathbf{r}) \qquad (59) \\ & + B^{ss\rho^\alpha}\,\mathbf{s}_q(\mathbf{r})\cdot\mathbf{s}_{q'}(\mathbf{r})\Big]\rho_0^\alpha(\mathbf{r}) , \qquad (60) \end{aligned}$$

$$\mathcal{E}^{\kappa\kappa\rho^\gamma} \;\equiv\; \int d^3r \sum_{q=p,n} A^{\tilde\rho\tilde\rho\rho^\gamma}\;\left|\tilde\rho_q(\mathbf{r})\right|^2\rho_0^\gamma(\mathbf{r})\,, \tag{61}$$

where the coupling constants A/B characterize terms in which the two linear densities involved refer to identical/different isospins. Note that neutron-proton pairing is not considered. Also, $\rho_0(\mathbf{r})$ is the isoscalar part of the matter density. As single-particle states have a definite isospin projection, $\rho_0(\mathbf{r}) = \rho_n(\mathbf{r}) + \rho_p(\mathbf{r})$.

In the present case, both neutron and proton particle numbers are restored. Doing so requires to consider two gauge angles φ_n and φ_p for neutrons and protons, respectively. As a result, PNR energies are obtained through

a double integration over the complex plane where the corresponding variables are denoted as z_n and z_p.

As far as the regularization of the bilinear part of the toy functional, see Sect. IV C 2, it still leads to the condition $A^{ss} = -A^{\rho\rho}$ and thus only constrains the like-particle interaction. Then, one notes that the pseudo matrix elements introduced in Eq. (52) to deal with the part of the EDF containing non-integer powers of the density matrices now depend on both the neutron z_n and proton z_p gauge variables because of the dependence on the isoscalar part of the transition local density in Eqs. (59-61). With the pseudo two-body matrix elements $\bar{v}^{\rho\rho\rho^\alpha}_{\mu\nu\mu\nu}[z_n, z_p]$ at hand, one can apply the correction formula of Eq. (43) of Paper II ensuring that the matrix elements are now placed underneath the integrals over the two gauge angles.

Once the part of the energy kernel $\mathcal{E}[z_n, z_p]$ that depends only on integer powers of the density matrix has been regularized, one is left with the spuriosities brought by the fractional power of the isoscalar transition density $\left[\rho_q^{1z_q}(\mathbf{r}) + \rho_{\bar{q}}^{1z_{\bar{q}}}(\mathbf{r})\right]^\alpha$. The branch cuts of the latter are not the same as those seen when dealing with a single particle species. This modifies the analysis but does not change the fact that the theory is not satisfactory, irrespective of the fine tuning done to define the integration contour. As a result, PNR energies cannot be made shift invariant and display smooth spurious steps as one changes the proton and/or neutron radii of integration or deforms the system along a certain degree of freedom.

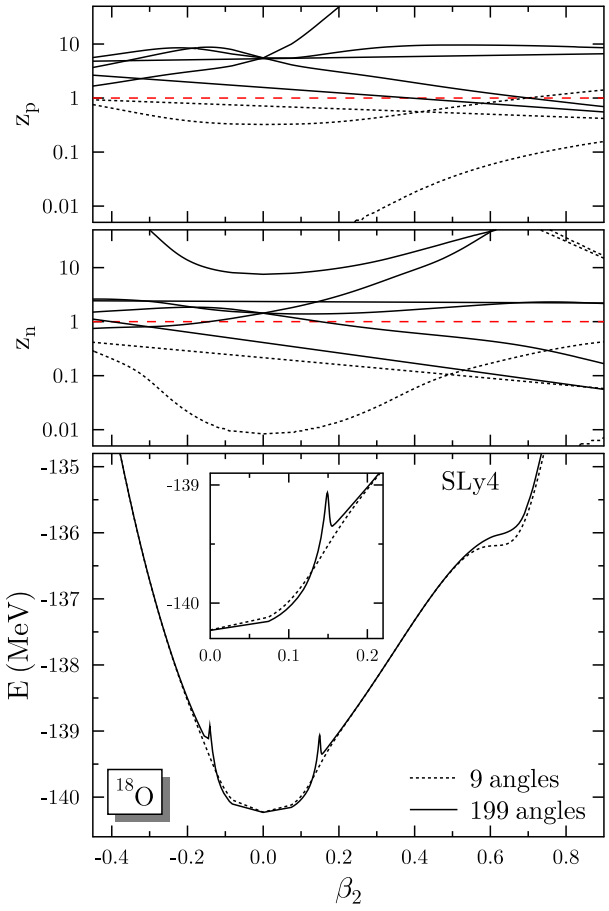

FIG. 8: (Color online) Spectrum of poles $z_\mu = |u_\mu/v_\mu|$ for protons (top panel) and neutrons (middle panel) as a function of quadrupole deformation, which for levels in the vicinity of the Fermi energy resembles a stretched and slightly distorted Nilsson diagram. The dashed red line at $z_q = 1$ denotes the radius of the standard integration-contour $R_q = 1$. The bottom panel shows the PNR energy $\mathcal{E}^N$ for two different numbers of discretization points in the computation of the integrals over the gauge neutron φ_n and proton φ_p angles.

V. APPLICATIONS

We wish to illustrate the analytical results obtained in the previous Sections through results of realistic calculations. We perform PNR calculations after variation of ^{18}O. We use the SLy4 parametrization [18] of the Skyrme EDF together with a pairing functional derived from a Delta Interaction (DI). The Coulomb exchange part of the functional, usually calculated in the Slater approximation, is omitted as done in Paper II. The SLy4 Skyrme parametrization includes a term of the type $\mathcal{E}^{\rho\rho\rho^{1/6}}$ which is perfectly suited to the present discussion.

A. Uncorrected calculations

As explained in Sect. III A, traditional PNR calculations have been performed using non-diagonal kernels defined through the prescription $\mathcal{E}[0, \varphi] \equiv \mathcal{E}[\rho^{0\varphi}, \kappa^{0\varphi}, \kappa^{\varphi 0\,*}]$, where $\mathcal{E}[\rho, \kappa, \kappa^*]$ is the single-reference EDF. Figure 8 shows the PNR energy $\mathcal{E}^N$ obtained in this way for ^{18}O and displayed as a function of quadrupole deformation. The calculation is repeated twice, using 5 and 199 points in the discretization of the integrals over the two gauge angles.

One observes that the deformation energy surface obtained with 5 integration points is smooth and looks physically reasonable. However, as one increases the number of integration points, divergences develop, precisely at deformations where a neutron or a proton single-particle state crosses the Fermi energy in the underlying SR states, i.e. when the associated non-integrable branch point crosses the unit circle in the complex plane. This is consistent with the discussion given in Sect. IV D 2 for the *uncorrected* SLy4 parametrization. Such divergences are at variance with the results obtained in Paper II with the SIII parametrization. Indeed, SIII is of specific functional form such that all the poles at $z = \pm z_\mu$ are simple poles. This is notably due to the fact that the trilinear terms entering SIII do not display products of three density matrices referring to the same isospin. As explain in Sect. IV B 3, this property leads to a finite Cauchy principle value as the poles cross the integration circle.

Still, the finite step left in the PNR energy as a

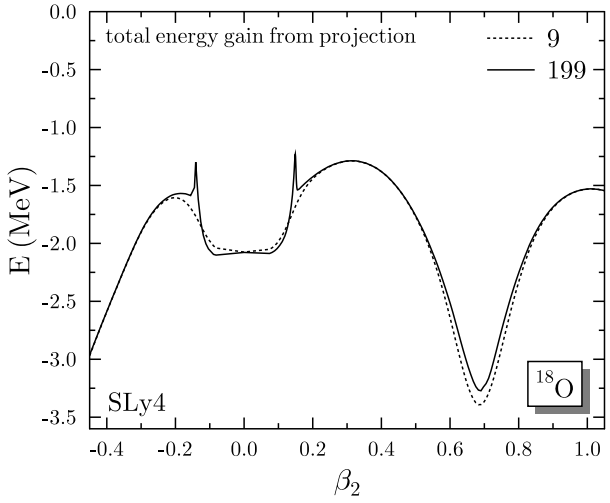

FIG. 9: Energy gain from particle number restoration as a function of quadrupole deformation for two different numbers of discretization points in the computation of the integrals over the gauge angles.

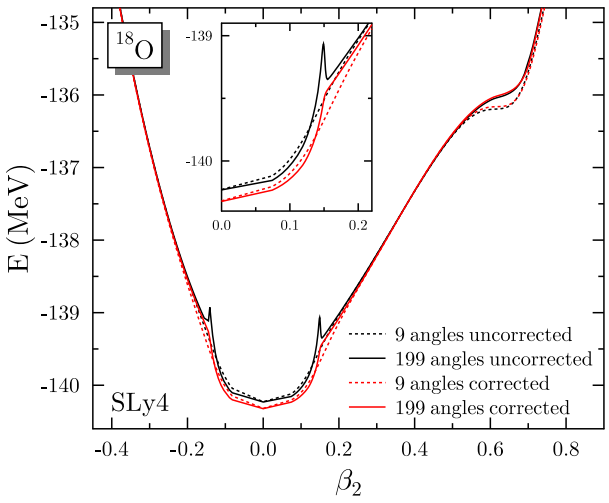

FIG. 10: (Color online) Particle number restored energy $\mathcal{E}^N$ as a function of quadrupole deformation without and with regularization of all bilinear terms in the EDF, including the quadratic part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$. Results are shown for two different numbers of discretization points in the computation of the integrals over the gauge angles.

pole/branch cut enters or leaves the integration circle is a pathology shared by the calculations performed with SLy4 and SIII. Those steps are better visible in Fig. 9 which displays the gain from particle number restoration with respect to the SR energy (rather than the absolute PNR binding energy) using SLy4. Note in passing that the reason why the structure around $\beta_2 = 0.7$ does not display a typical step can be understood from the fact that two pairs of levels cross the Fermi energy at that deformation, as discussed in Paper II.

By looking carefully, one can observe an interesting difference between the steps produced by SIII (see Paper II) and those obtained presently using SLy4. The steps generated by SLy4 are significantly less steep than those produced by SIII. This is because, whereas a sharp step is generated by an isolated pole leaving or entering the integration circle in the case of SIII, which occurs over an infinitesimal interval of deformation, it is generated by a branch cut leaving or entering the integration circle in the case of SLy4, which happens over a finite interval of deformation.

B. Correcting the bilinear part

The specificity of SLy4 is to contain a term of the type $\mathcal{E}^{\rho\rho\rho^{1/6}}$. As discussed in Sect. IV C, one could have hoped that regularizing the quadratic part of this term through the correction method proposed in Paper I would lead to a well-behaved PNR energy; i.e. that the remaining fractional power of the density would not create any pathology, in particular in view of the fact that the branch point becomes integrable in this case. Of course, it is important to remember that the correction method proposed in Paper I relies on solid basis only for terms of the form $\mathcal{E}^{\rho^n}$, with n integer. Thus, regularizing the quadratic part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$ in this way is purely empirical.

As a matter of fact, the results displayed in Fig. 10 demonstrate that proceeding to such a correction does not lead to a well-behaved PNR energy. The integrability of the branch points remaining after regularizing the quadratic part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$ is such that all the divergences have disappeared. This is a necessary but not sufficient condition to obtain a well-behaved PNR energy. Indeed, Fig. 11 clearly demonstrates that the spurious steps are still present and have in fact not been reduced by regularizing the bilinear part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$. In addition, one observes that the corrected results still depend strongly on the discretization of the integrals over the gauge angles. More precisely, all terms of the energy functional that are strictly bilinear have become independent on the number of discretization points whereas the term with the extra fractional power is not. Considering the experience we have gathered about well-behaved PNR energies, such a dependence is a fingerprint of a ill-defined PNR theory.

As discussed in Sect. IV D 2, Figs. 10 and 11 also show that regularizing the quadratic part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$ leads to the replacement of divergences by non-derivable points in the PNR potential energy curve. Indeed, kinks are clearly visible at the deformation where the divergences appeared before applying the correction method. Using more mesh points for Q_{20}, φ_p and φ_n, one could resolve even better the non-derivable character of the energy as a branch point passes through the integration circle. This pattern relates directly to the analytical result obtained in Eq. (58).

Finally, note that it is a particularity of the SLy4 interaction complemented with the pairing interaction

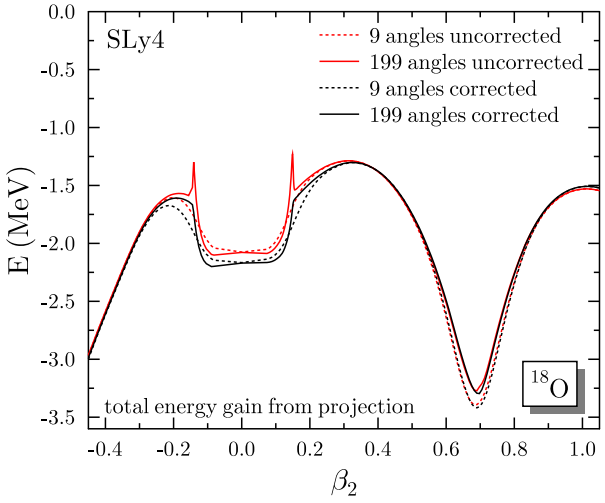

FIG. 11: (Color online) Energy gain from PNR as a function of quadrupole deformation without and with regularization of all bilinear terms in the EDF, including the quadratic part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$. Results are shown for two different numbers of discretization points in the computation of the integrals over the gauge angles.

chosen here that the combined correction of all density-independent terms is always very small in ^{18}O, often even difficult to resolve on the plots.

C. Shift transformation

The finite steps that arise in the deformation energy surface are a reminiscence of the violation of the shift invariance of the PNR energy. Such a violation is unambiguously demonstrated by varying the radius of the integration contour in Eq. (55); i.e. by computing Eq. (58) as a function of R.

The upper panel of Fig. 12 shows the PNR energy of ^{18}O at a deformation $Q_{20} = 600$ fm^2, obtained using the SLy4 parametrization. The energy is displayed as a function of the radius of the integration contour used to restore the proton number. The radius for the neutrons is $R_n = 1$ in all cases. The calculation is performed with and without a regularization of the bilinear part of the functional and for two different numbers of integration points (taken to be the same for protons and neutrons). Finally, the bottom panel of Fig. 12 shows the same quantity obtained from the SIII parametrization at a quadrupole deformation $Q_{20} = 500$ fm^2.

The upper panel of Fig. 12 confirms that, even after regularizing the bilinear part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$, the PNR energy is not invariant under shift transformation. Even though the correction method does remove the divergence, it does not eliminate the shaped steps as the integration contour goes through a branch cut. In addition, both the corrected and uncorrected PNR energies depends strongly on the discretization of the integrals.

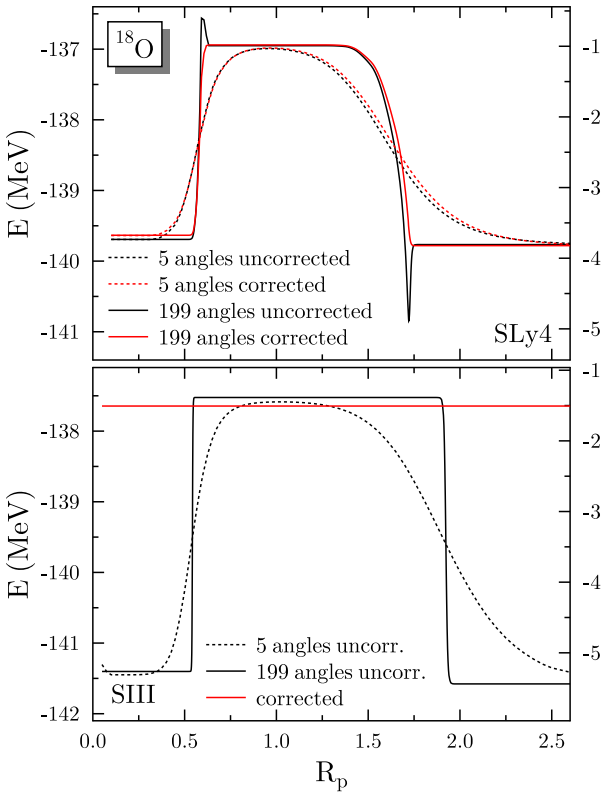

FIG. 12: (Color online) Particle-number restored energy $\mathcal{E}^N$ as a function of the radius R_p of the contour chosen to restore proton number ($R_n = 1$) and for two different numbers of discretization points in the computation of the integrals over the gauge angles. Results are shown before and after regularization of the bilinear part of the EDF. Upper panel: at a prolate quadrupole deformation $Q_{20} = 600$ fm^2 using the SLy4 parametrization. Bottom panel: at a prolate quadrupole deformation $Q_{20} = 500$ fm^2 using the SIII parametrization. The corrected SIII curve is independent on the number of discretization point; hence, only one curve is shown. The left scale shows the absolute value of the binding energy whereas the right scale shows the energy gain from symmetry restoration.

Again, those two features are entirely due to the term in the functional depending on a non-integer power of the density. After regularization, all terms that are strictly bilinear become shift invariant. For comparison, the bottom panel of Fig. 12 shows the PNR energy obtained with SIII in Paper II. We recall that SIII contains only linear, bilinear and trilinear terms which are such that all poles at $z = \pm z_\mu$ are of order one. The corresponding PNR energy is, after regularization, independent on the contour and the number of discretization points with a numerical precision better than 1 keV. When restoring the particle number that the SR-EDF calculation was constrained to, the finite spurious contributions are the smallest when using a circle radius close to $R = 1$ for the reasons outlined in Paper II. Consequently, the corrected value is rather close to the uncorrected one in such a case.

It is fortuitous that for the deformation $Q_{20} = 500$ fm^2 in ^{18}O and when using SLy4 the combined correction of all density-independent terms is very small, such that corrected and uncorrected curves are close at very small values of R_p in Fig. 12 and even cannot be distinguished within the resolution of the plot for larger R_p shown.

Just as for the deformation energy curve as a function of quadrupole deformation, one observes, by comparing the two panels of Fig. 12, that the steps generated by SLy4 are significantly less steep than those produced by SIII before correction (calculated in both cases with enough integration points to resolve them). This is due to the fact that the steps are generated by a single pole leaving or entering the integration circle in the case of SIII, which occurs over an infinitesimal variation of R_p, whereas they are generated by a branch cut leaving or entering the integration contour in the case of SLy4, which happens over a finite interval of variation of R_p.

Just as for the behavior of the deformation energy curve as a function of quadrupole deformation, the curves obtained with 199 integration points in the upper panel of Fig. 12 show that the divergences seen before regularizing the quadratic part of $\mathcal{E}^{\rho\rho\rho^{1/6}}$ have been replaced by cusps. Using more mesh points for R_p and φ_p, one could resolve even better the non-derivable character of the PNR energy as the integration circle passes the branch points. This is a direct illustration of the analytical result obtained in Eq. (58) and is schematically displayed in Fig. 7.

An important byproduct of the previous result is that they invalidate PNR calculations performed using a fully antisymmetrized two-body interaction that depends on the medium through a fractional power of the density, e.g. the Gogny interaction. The problem was further circumvented in Ref. [3] by using the projected density in place of the transition density in the density-dependent term of the Gogny interaction. However, such a procedure singles out one density factor in the energy kernel in a way that seems highly arbitrary and not easily extendable to more involved EDFs. In addition, such a prescription of using the correlated density into the density-dependent term of the effective vertex leads to unsatisfactory results for other multi-reference calculations; e.g. calculations including parity restoration and configuration mixing along the octupole degree of freedom [19].

VI. SUMMARY AND CONCLUSIONS

In Ref. [1], pathologies of calculations aiming at restoring particle number and performed within the Energy Density Functional (EDF) framework have been highlighted. In Ref. [5], the first paper of the present series, we demonstrated that such pathologies are in fact shared by all multi-reference (MR) calculations, i.e. symmetry restoration and/or Generator Coordinate Method (GCM)-based configuration mixing calculations, performed within the EDF framework. In Ref. [5], a formal and practical solution that applies (i) to any symmetry restoration and/or GCM-based configuration mixing calculation (ii) to EDFs depending only on integer powers of the density matrices, was proposed. In Ref. [6], the second paper of the present series, the regularization method was applied to Particle Number Restoration (PNR) calculations using an energy functional that depends only on integer powers of the density matrices; e.g. which contains linear, bilinear and trilinear terms.

The limitation of the correction method proposed in Ref. [5] to energy functionals depending on integer powers of the density matrices is a critical feature as most functionals found in the literature contain non-integer powers of the (normal) density matrix, both in the functional modeling the strong interaction and in the functional modeling the Coulomb interaction, due to the Slater approximation to the exchange term [9]. Such non-integer powers of the density matrices pose difficulties which go beyond those posed by integer powers: as transition densities are complex, taking their non-integer powers amounts to dealing with a multivalued function on the complex plane. This makes the analysis of the associated pathologies more involved.

In the present paper, the third of the series, the viability of non-integer powers of the density matrices has been addressed, building upon the analysis already carried out in Ref. [1]. First, we proposed to reduce the pathological character of terms depending on a non-integer power of the density matrices by regularizing the fraction that relates to the integer part of the exponent, using the method proposed in Ref. [5]. This amounts to scaling down the extent of the problem to the one potentially encountered using a fully antisymmetrized effective interaction depending further on a fractional power of the density; e.g. the Gogny force. Second, we discussed in detail the spurious character of the remaining fractional power of the density (matrix). Both through analytical derivations and numerical applications (using the SLy4 Skyrme parametrization), we demonstrated that regularizing the fraction related to the integer part of the exponent does remove divergences in the particle number restored energy but replace them by cusps which are as unphysical as the original divergences. In addition, the spurious steps in the PNR energy and the related breaking of shift invariance prevail. Such results thus invalidate PNR calculations performed using a fully antisymmetrized two-body interaction that depends on the medium through a fractional power of the density.

Eventually, and because we do not see any well-defined basis to correct the corresponding pathologies, we conclude at this point that non-integer powers of the density matrices are not viable and should be avoided in the first place when constructing nuclear energy density functionals to be used in MR-EDF calculations in the future. However, one will have to restrict the form to rather low integer orders in the density matrices. For example, the EDF recently proposed by Baldo *et al.* [20] includes terms up to fifth power in the total density $\rho(\mathbf{r})$, which

lead to self-interaction terms [21] that will require a regularization containing quadruple sums over single-particle states, which will be too costly in realistic calculations.

Let us make an additional comment regarding the drastic conclusion to discard non-integer powers of the density matrices altogether. On the one hand, integer powers of the density matrices appear naturally when constructing the EDF through ab-initio calculations, e.g. through many-body perturbation theory. On the other hand, non-integer powers of the density matrices, if not introduced merely on phenomenological grounds, do often, if not always, result from interpreting integrals over momenta up to k_F providing the infinite matter equation of state with contributions of the kind k_F^n as density-dependent term through the use of $k_F \sim \rho^{1/3}$. Transported to finite nuclei, where the latter relationship has no rigorous basis, through some version of the local density approximation, this leads to an EDF that contains terms of the form $\rho^{n/3}$. Although such a constructive procedure of the nuclear EDF does not lead to particular problems in single reference (SR) calculations, it does so when this procedure is extended to MR calculations as even the local part of the scalar-isoscalar transition density matrix is complex, stretching one step too far the above procedure proceeding through infinite matter and the use of $k_F \Leftrightarrow \rho^{1/3}$. Finally, there are both practical reasons and formal motivations to conclude that (i) non-integer powers of the density (matrix) are not viable in (multi-reference) EDF calculations (ii) parameterizations making only use of integer powers of the densities need to be constructed in the very near future. Last but not least, note that such a conclusion actually extends to any form of the EDF that generates branch cuts when continued over the complex.

Acknowledgments

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