Formulation of functional theory for pairing with particle number restoration

Guillaume Hupin,[1,*] Denis Lacroix,[1,†] and Michael Bender[2,3,‡]

[1]*Grand Accélérateur National d'Ions Lourds (GANIL), CEA/DSM-CNRS/IN2P3, Bvd Henri Becquerel, F-14076 Caen, France*

[2]*Université Bordeaux, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*

[3]*CNRS/IN2P3, Centre d'Etudes Nucléaires de Bordeaux Gradignan, UMR5797, F-33175 Gradignan, France*

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The restoration of particle number within energy density functional theory is analyzed. It is shown that the standard method based on configuration mixing leads to a functional of both the projected and nonprojected densities. As an alternative that might be advantageous for mass models, nuclear dynamics, and thermodynamics, we propose to formulate the functional in terms directly of the one-body and two-body density matrices of the state with good particle number. Our approach does not contain the pathologies recently observed when restoring the particle number in an energy density functional framework based on transition density matrices and can eventually be applied with functionals having arbitrary density dependencies.

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I. INTRODUCTION

Energy density functional (EDF) methods provide a universal framework to describe nuclear structure, nuclear dynamics, or thermodynamics. Tremendous advances have been made in the last few decades on the practical application of EDF methods to nuclei [1]. Still, despite their long success, some of the fundamental assumptions made to justify the usual strategies of how the EDF techniques are constructed and used for nuclear systems have not yet been satisfactorily clarified. Most, if not all, EDF approaches break as many symmetries of the nuclear Hamiltonian as possible: translational, rotational, and U(1) symmetry in gauge space are among the most important ones. In fact, the exploitation of symmetry breaking in nuclei is strongly motivated by experimental observations. For instance, the appearance of highly collective rotational bands in spectroscopic data clearly points to the existence of deformed intrinsic states in many nuclei [2]. Similarly, there is evidence that pairing can be often treated by explicitly breaking the U(1) gauge symmetry of eigenstates of the particle number operator, as, for instance, in a Bardeen-Cooper-Schrieffer (BCS) or Hartree-Fock-Bogoliubov (HFB) approach [2,3]. Nuclei are, however, finite systems and methods like BCS or HFB do not properly treat quantum fluctuations of the order parameter associated with the broken symmetry [3]. These fluctuations can be incorporated either by a statistical treatment of the order parameter or by the restoration of the relevant symmetry [3]. The concept of symmetry breaking and restoration stands out as the tool of choice within the EDF framework.

It has, however, been recently shown that restoration of symmetries has to be handled with great care in an EDF framework [4–7]. In particular, the configuration mixing within a multi-reference (MR) EDF approach might lead to serious practical difficulties that can, however, eventually be cured [6,8]. Besides compromising applications, these difficulties have clearly pointed out the necessity to clarify the theoretical framework on which the theory can be build.

The discussion in the present paper is restricted to ground-state properties and to particle number projection, for which detailed analyses have been recently made. This case is the simplest situation in which pathologies of the MR-EDF approach have been observed [4], analyzed, and regularized [6,8]. The first goal of the present work is to provide an alternative analysis of the EDF theory using configuration mixing to restore symmetries without and with the regularization. It will be shown that neither the nonregularized nor the regularized functionals can straightforwardly be interpreted in terms of the densities of projected or nonprojected states. Starting from this analysis, the second intent of this work is to propose an alternative way to introduce a functional theory that is U(1) symmetry conserving, and that without making use of the multi-reference technique. Our approach remains close to the Hohenberg-Kohn [9] and Kohn-Sham [10] framework and uses a projected state as an intermediate trial state to construct the components of the functional. This approach avoids the difficulties recently encountered in MR-EDF approaches and can be applied also with functionals that cannot be safely employed within the standard MR-EDF approach, as for example functionals with nonanalytical density dependences.

II. PARTICLE NUMBER RESTORATION WITHIN EDF THEORY: STANDARD APPROACH

The strategy to obtain a functional for pairing including particle number restoration has been extensively analyzed recently [5,6,8,11], and we only give here the main steps necessary for our discussion. Following these references, in this section we will consider a specific class of functional form that will be sufficient for the present discussion.[1] At the

*hupin@ganil.fr
†lacroix@ganil.fr
‡bender@cenbg.in2p3.fr

[1]Note that none of the currently used SR-EDF functionals belong to this class, because they have nonanalytical density dependences. The form (1) is the only one (restricting ourselves here to bilinear functionals) for which the recently proposed regularization applies.

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so-called single-reference (SR) level, a quasi-particle (QP) vacuum of Bogoliubov type $|\Phi_0\rangle$ is used to construct the normal and anomalous density matrices, denoted by ρ and κ, that serve to construct the functional. The energy is then written as

$$\begin{aligned}\mathcal{E}_{\rm SR}[\Phi_0] &= \mathcal{E}_{\rm SR}[\rho,\kappa,\kappa^*] \\ &= \sum_i t_{ii}\rho_{ii} + \frac{1}{2}\sum_{i,j}\overline{v}^{\rho\rho}_{ijij}\rho_{ii}\rho_{jj} + \frac{1}{4}\sum_{i,j}\overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}\kappa^*_{i\bar{i}}\kappa_{j\bar{j}}\,,\end{aligned} \tag{1}$$

where $\overline{v}^{\rho\rho}$ and $\overline{v}^{\kappa\kappa}$ denote the effective vertices in the particle-hole and particle-particle channels. Standard SR-EDF can be schematically seen as the sequence

$$\Phi_0 \Longrightarrow (\rho,\kappa,\kappa^*) \Longrightarrow \mathcal{E}_{\rm SR}. \tag{2}$$

The price to be paid for incorporating pairing with a rather simple functional is to use an intermediate state $|\Phi_0\rangle$ that is not an eigenstate of particle number. In a second step, the symmetry can be restored projecting out the component with N particles

$$|\Psi_N\rangle = P^N|\Phi_0\rangle, \tag{3}$$

where P^N denotes the particle number projection operator defined through [2,3]

$$P^N = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\ e^{i\varphi(\hat{N}-N)}. \tag{4}$$

The expectation value of any operator O that conserves particle number can then be expressed as

$$\frac{\langle\Psi_N|\,O\,|\Psi_N\rangle}{\langle\Psi_N|\Psi_N\rangle} = \int_0^{2\pi} d\varphi\ \frac{\langle\Phi_0|O|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle}\mathcal{N}_N(0,\varphi)\,, \tag{5}$$

where the shorthand

$$\mathcal{N}_N(0,\varphi) \equiv \frac{e^{-i\varphi N}}{2\pi}\frac{\langle\Phi_0|\Phi_\varphi\rangle}{\langle\Psi_N|\Psi_N\rangle} \tag{6}$$

has been introduced. Here φ denotes the gauge angle, whereas $|\Phi_\varphi\rangle = e^{i\varphi\hat{N}}|\Phi_0\rangle$ refers to the state $|\Phi_0\rangle$ rotated in gauge space. The kernel entering in the integral of Eq. (5) corresponds to the transition matrix element of an operator between two quasi-particle vacua. One can then take advantage of the generalized Wick's theorem (GWT) [2,12] to express the kernel in terms of the transition density matrices

$$\rho^{0\varphi}_{ij} \equiv \frac{\langle\Phi_0|a^\dagger_j a_i|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle}, \tag{7}$$

$$\kappa^{0\varphi}_{ij} \equiv \frac{\langle\Phi_0|a_j a_i|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle}, \tag{8}$$

$$\kappa^{\varphi 0\star}_{ji} \equiv \frac{\langle\Phi_0|a^\dagger_i a^\dagger_j|\Phi_\varphi\rangle}{\langle\Phi_0|\Phi_\varphi\rangle}. \tag{9}$$

For instance, when O is a two-body Hamiltonian, the two-body interaction $\overline{v}$ entering in Eq. (5) takes a form similar to Eq. (1) with $\overline{v}^{\rho\rho} = \overline{v}^{\kappa\kappa} = \overline{v}$ and where the densities ρ and κ are replaced by the corresponding transition densities, Eqs. (7)–(9). Guided by the Hamiltonian case, the energy functional associated with particle number restoration is usually defined through

$$\mathcal{E}_N[\Psi_N] \equiv \int_0^{2\pi} d\varphi\ \mathcal{E}_{\rm SR}[\rho^{0\varphi},\kappa^{0\varphi},\kappa^{\varphi 0\star}]\mathcal{N}_N(0,\varphi)\,. \tag{10}$$

This energy functional is a special case of a so-called multi-reference EDF (MR-EDF).

The present strategy to restore symmetries in an EDF framework deserves some further remarks: First, expression (10) is postulated having in mind the Hamiltonian case. However, the MR-EDF theory should not be confounded with the expectation value of a Hamilton operator. In particular, an energy functional has much more flexibility regarding the functional form of the energy kernels in Eq. (10), which can be used for the efficient modeling of in-medium correlations. Second, the construction of the MR-EDF, Eq. (10), from the SR-EDF by simply replacing the normal and anomalous density matrices in the SR-EDF by the corresponding transition density matrices is postulated by analogy to the GWT. While it appears rather natural, it was shown recently that this strategy to construct the MR-EDF might lead to an ill-defined functional that exhibits divergencies and jumps in practical applications [5,6,8]. While a solution to this problem has been proposed and applied in Refs. [6,8], a consistent framework for MR-EDF approaches is still missing. A clear illustration of this is the ongoing debate about which densities should enter in the functional [13], as well as the recently recognized impossibility to use noninteger powers of the transition density in MR energy functionals [11].

The very notion of symmetry restoration within an EDF framework remains to be clarified. For instance, it has been shown recently [7] that also regularized MR energy functionals may in general not transform as an irreducible representation of the restored symmetry, unless additional constraints are introduced.

In the present section, we will further analyze the way the MR-EDF is constructed and the possible sources of difficulties. For simplicity, we restrict ourselves to a case where the two-body effective interaction kernels entering Eq. (1) are *independent of the densities*.

A peculiarity of particle number projection is that the canonical bases of the original state $|\Phi_0\rangle$ and of the rotated states $|\Phi_\varphi\rangle$ are the same when making a suitable choice of the Bogoliubov transformation between quasi-particle operators of these states. Accordingly, the canonical base of the projected state $|\Psi_N\rangle$ is also the same as the one of the original reference state $|\Phi_0\rangle$. In the following, we will implicitly assume that densities are written in this canonical basis in which we have

$$\rho^{0\varphi}_{ij} = \delta_{ij}n^{0\varphi}_i, \quad \kappa^{0\varphi}_{ij} = \delta_{j\bar{i}}\kappa^{0\varphi}_{i\bar{i}}, \quad \kappa^{\varphi 0\star}_{ij} = \delta_{j\bar{i}}\kappa^{\varphi 0\star}_{i\bar{i}}, \tag{11}$$

whereas the energy $\mathcal{E}_N$ takes the form

$$\begin{aligned}\mathcal{E}_N[\Psi_N] = &\sum_i t_{ii}\int_0^{2\pi} d\varphi n^{0\varphi}_i\mathcal{N}_N(0,\varphi) \\ &+ \frac{1}{2}\sum_{i,j}\overline{v}^{\rho\rho}_{ijij}\int_0^{2\pi} d\varphi n^{0\varphi}_i n^{0\varphi}_j\mathcal{N}_N(0,\varphi) \\ &+ \frac{1}{4}\sum_{i,j}\overline{v}^{\kappa\kappa}_{i\bar{i}j\bar{j}}\int_0^{2\pi} d\varphi\kappa^{\varphi 0\star}_{i\bar{i}}\kappa^{0\varphi}_{j\bar{j}}\,\mathcal{N}_N(0,\varphi)\,.\end{aligned} \tag{12}$$

After a lengthy but straightforward calculation, the energy functional can be expressed as

$$\mathcal{E}_N[\Psi_N] = \sum_i t_{ii} n_i^N + \frac{1}{2}\sum_{i,j,j\neq\bar{\imath}} \overline{v}^{\rho\rho}_{ijij} R^N_{ijij} + \frac{1}{4}\sum_{i\neq j, i\neq\bar{\jmath}} \overline{v}^{\kappa\kappa}_{i\bar{\imath}j\bar{\jmath}} R^N_{j\bar{\jmath}i\bar{\imath}} + \frac{1}{2}\sum_i \overline{v}^{\rho\rho}_{i\bar{\imath}i\bar{\imath}} \int_0^{2\pi} d\varphi n_i^{0\varphi} n_i^{0\varphi} \mathcal{N}_N(0,\varphi) + \frac{1}{2}\sum_i \overline{v}^{\kappa\kappa}_{i\bar{\imath}i\bar{\imath}} \int_0^{2\pi} d\varphi \kappa_{i\bar{\imath}}^{\varphi 0\star} \kappa_{i\bar{\imath}}^{0\varphi} \mathcal{N}_N(0,\varphi), \quad (13)$$

where n_i^N are the occupation numbers

$$n_i^N \equiv \frac{\langle\Psi_N|a_i^\dagger a_i|\Psi_N\rangle}{\langle\Psi_N|\Psi_N\rangle}, \quad (14)$$

and R^N_{ijkl} corresponds to the two-body density matrix

$$R^N_{ijkl} \equiv \frac{\langle\Psi_N|a_k^\dagger a_l^\dagger a_j a_i|\Psi_N\rangle}{\langle\Psi_N|\Psi_N\rangle} \quad (15)$$

of the projected state. They can be expressed in terms of the gauge angle integrals as

$$n_i^N = \int_0^{2\pi} d\varphi\, n_i^{0\varphi} \mathcal{N}_N(0,\varphi), \quad (16)$$

and

$$R^N_{ijkl} = (\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}) \int_0^{2\pi} d\varphi n_i^{0\varphi} n_j^{0\varphi} \mathcal{N}_N(0,\varphi) + \delta_{j\bar{\imath}}\delta_{l\bar{k}} \int_0^{2\pi} d\varphi \kappa_{i\bar{\imath}}^{\varphi 0\star} \kappa_{k\bar{k}}^{0\varphi} \mathcal{N}_N(0,\varphi). \quad (17)$$

Equation (13) is rather enlightening with respect to the physical content of present MR-EDF calculations. Indeed, if one neglects the last two terms in Eq. (13), one sees that the functional associated with the projected state can be regarded as a functional of the one- and two-body components of this very state. Similarly, if one uses the same effective interaction $\overline{v}^{\rho\rho} = \overline{v}^{\kappa\kappa}$, then the last two terms of Eq. (13) recombine, and the two-body component $R^N_{i\bar{\imath}i\bar{\imath}}$ can be recognized, thanks to the relation

$$R^N_{i\bar{\imath}i\bar{\imath}} = n_i^N = \int_0^{2\pi} d\varphi \left(n_i^{0\varphi} n_i^{0\varphi} + \kappa_{i\bar{\imath}}^{\varphi 0\star} \kappa_{i\bar{\imath}}^{0\varphi}\right) \mathcal{N}_N(0,\varphi). \quad (18)$$

However, when using different effective vertices $\overline{v}^{\rho\rho} \neq \overline{v}^{\kappa\kappa}$ in the particle-hole and particle-particle channels, or when using vertices $\overline{v}^{\rho\rho}$ or $\overline{v}^{\kappa\kappa}$ that cannot be written as an antisymmetrized matrix elements of the two-body force, then the identification of the energy as a functional of one- and two-body density matrices of the projected state cannot be made anymore. Instead, it can only be written as a functional of the transition density matrices.[2] This subtlety is intimately connected to the presence of pathologies encountered in MR-EDF calculations. Indeed, the last two terms in Eq. (13) are nothing but the ones at the heart of the difficulties to construct a well-defined MR-EDF theory. As discussed in Refs. [5,8], for near-orthogonal states $\langle\Phi_0|\Phi_\varphi\rangle \simeq 0$, there is at least one $n_i^{0\varphi}$ and the corresponding $\kappa_{i\bar{\imath}}^{\varphi 0\star}$ and $\kappa_{i\bar{\imath}}^{0\varphi}$ that all go to infinity. As a consequence, the two terms can separately become larger than any physical scale in the nucleus. They do, however, recombine to a well-behaved expression when a Hamiltonian is used, i.e., when $\overline{v}^{\rho\rho} = \overline{v}^{\kappa\kappa}$. Without taking specific care of these terms in the restoration of symmetry within the functional framework, there is a spurious contribution that leads to discontinuities and divergences when plotting the particle number projected energy as a function of a collective coordinate.

A. MR-EDF theory with regularization

A strategy to construct a well-behaved MR-EDF theory proposed in Refs. [6,8] is to remove terms that might not properly recombine in the MR-EDF approach in such a way that the spurious contamination is removed without touching the physical content of the functional. The resulting functional then takes the form (technical details are given in Appendix A)

$$\mathcal{E}_N[\Psi_N] = \sum_i t_{ii} n_i^N + \frac{1}{2}\sum_{i,j,j\neq\bar{\imath}} \overline{v}^{\rho\rho}_{ijij} R^N_{ijij} + \frac{1}{4}\sum_{i\neq j, j\neq\bar{\imath}} \overline{v}^{\kappa\kappa}_{i\bar{\imath}j\bar{\jmath}} R^N_{j\bar{\jmath}i\bar{\imath}} + \frac{1}{2}\sum_i \overline{v}^{\rho\rho}_{i\bar{\imath}i\bar{\imath}} \left(n_i^N n_i^N - \delta n_i \delta n_i\right) + \frac{1}{2}\sum_i \overline{v}^{\kappa\kappa}_{i\bar{\imath}i\bar{\imath}} \left[n_i^N\left(1 - n_i^N\right) + \delta n_i \delta n_i\right], \quad (19)$$

where $\delta n_i = n_i^N - n_i^0$ is the difference between the occupation number of the level i in the projected and the nonprojected state.

Expression (19) is of particular interest for the following discussion regarding the construction of energy functional theory. First, let us remark that compared to the previous form (13), the gauge-space integrals are now hidden in the components of the one- and two-body density matrices of the projected state. In addition, the last two lines of Eq. (19) are also functionals of the occupation numbers n_i^0 in the original nonprojected state. The analysis of the regularization procedure to remove spurious contributions to the MR-EDF method [6,8,11] suggests that these terms will always be well behaved.

An example of a deformation energy curve obtained from a particle number projected MR-EDF calculation with the Skyrme interaction SIII and a pairing functional of volume type is shown in Fig. 1 (dashed line). The MR-EDF is numerically calculated using expression (10) and the Fomenko discretization procedure of the gauge-space integrals described, for instance, in Ref. [8]. Here, 199 discretization points have been used. This large number is necessary to resolve the discontinuities that stem from the spurious contribution to the nonregularized MR-EDF [8]. As in Ref. [8], the Lipkin-Nogami procedure is used in the

[2] We recall that the expectation value of the two-body operator in a projected state can be written as a functional of the two-body density of this state or, fully equivalently, as a functional of the one-body density matrices. This property does not hold for general functionals that are constructed without reference to an underlying Hamiltonian.

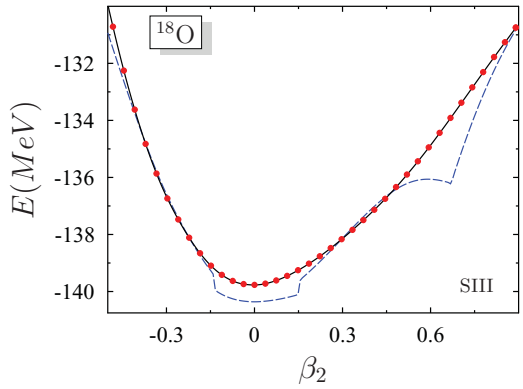

FIG. 1. (Color online) Particle number restored deformation energy curve of ^{18}O as a function of quadrupole deformation β_2 and calculated within standard MR-EDF technique using projection after variation (PAV) with SIII and a delta pairing interaction before (blue dashed curve) and after (black solid curve) regularization. The red filled circles correspond to the results obtained using directly Eq. (19) (see text). To compare with previous work [8], the Coulomb exchange contribution has been subtracted from the energy.

minimization of the energy of the state $|\Phi_0\rangle$. The solid line corresponds to the MR-EDF method with the regularization proposed in Ref. [6]. In this figure, we also show the results (filled circles) obtained using directly the expression (19) that has been proven above to be analytically equivalent to the regularized MR-EDF functional. Note that, in the latter case, we have used a method called hereafter the "recurrence method" to compute the projected occupation numbers and components of the projected two-body densities. This method is described in detail in Appendix B. Although the use of gauge angle integration would have given exactly the same results, this method has the advantage of being very simple and numerically efficient and of not making use of transition density matrices. As expected, the energy obtained with expression (19) exactly matches the one obtained using the regularized MR-EDF functional. This formulation provides a new and alternative insight into the content of particle number restored energy functionals.

B. Critical analyses of standard method

As discussed above, specific regularizations in MR-EDF functionals are needed to avoid discontinuities such as the jumps appearing in Fig. 1. At this point, even with the regularization, two important problems remain:

(i) Terms that have a nonanalytical density dependence, for example, a noninteger power such as often used in parametrizations of the Skyrme and Gogny interactions, cannot be regularized with the procedure proposed in Ref. [6]. Indeed, the functional itself becomes in that case multivalued in the complex plane and cannot be properly defined [5,11].

(ii) A second issue illustrated in Eq. (19) is that the last two terms are not only a functional of the occupation numbers of the projected state, but also of the occupation probabilities of the original reference state $|\Phi_0\rangle$. Accordingly, the energy remains a functional of the density of the quasi-particle vacuum that is not an eigenstate of particle number. This raises the question of which density, i.e., projected, transition, or nonprojected, can be used to construct a functional for MR calculations.

In the following, we show that both (i) and (ii) can eventually be avoided by changing the strategy to construct the functional for pairing that accounts for particle number restoration.

III. EDF THEORY FOR PAIRING WITH PARTICLE NUMBER RESTORATION

Let us now discuss the critique (ii) made above concerning the components of the projected energy functional. In most functional approaches, an intermediate state is introduced to construct densities that are used to minimize the energy. This is the case in the usual DFT or at the SR-EDF level where the trial state is a Slater determinant or a quasi-particle vacuum. When restoring the symmetry in a MR-EDF framework, then, according to Eq. (19), the projected state can be *almost* regarded as an intermediate many-body state from which the one- and two-body density matrices used to define the functional are obtained.

However, due to the presence of n_i^0 in the energy, this functional happens to depend on components not only of the projected state, but also of the original reference state. A slight modification, however, can easily restore the unique dependence of the functional on the projected state. If, for instance, the following replacements

$$\begin{aligned} \left(n_i^N n_i^N - \delta n_i \delta n_i\right) &\Longrightarrow n_i^N n_i^N, \\ \left[n_i^N \left(1 - n_i^N\right) + \delta n_i \delta n_i\right] &\Longrightarrow n_i^N \left(1 - n_i^N\right), \end{aligned} \tag{20}$$

are made in Eq. (19), then the strategy of standard DFT to construct the EDF as a functional of the density of an auxiliary state, the projected state here, is recovered.[3]

The use of a projected product state as an auxiliary state has the advantage that it allows us to treat pairing in a particle number conserving framework. An illustration of a result obtained taking into account this modification in Eq. (19) is shown in Fig. 2 and compared to the original curve. This figure illustrates that the small change in the functional does not significantly modify the energy landscape. This is indeed not unexpected, since the difference δn_i (respectively $\delta n_i \delta n_i$) is likely to be much smaller than n_i^N (respectively $n_i^N n_i^N$).

By making the simple modification (20), the EDF framework can now be interpreted as a functional of the projected-state densities. Indeed, the state with good particle number can

[3]This does not mean, however, that we recover a theory that is equivalent to DFT. Indeed, at this stage, the functional (19) is still a functional of the two-body density matrix. However, as will be discussed below, for the specific case of particle number projection, the two-body density matrix is itself a functional of the one-body density matrix.

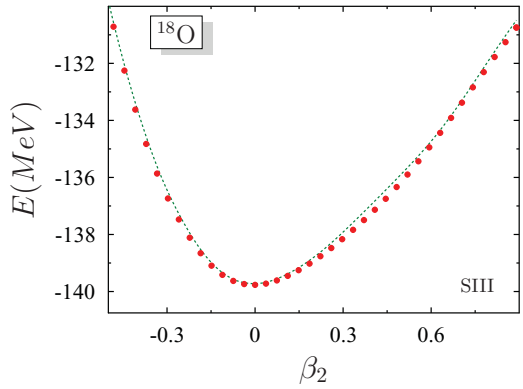

FIG. 2. (Color online) Particle number restored deformation energy surface of ^{18}O calculated using Eq. (19). The dotted curve is obtained by making the replacement (20) in Eq. (19).

now be regarded as the auxiliary many-body state that provides the quantities used to construct the EDF. Similar to Eq. (2), the corresponding theory can be regarded as a new sequence

$$\Psi_N \Longrightarrow (\rho^N, R^N) \Longrightarrow \mathcal{E}_N. \tag{21}$$

We note in passing that the slight modification (20) does not break the shift invariance of the energy functional discussed in Refs. [5,8]. At this point, let us make a few further important remarks:

(i) The functional form (19) is not completely surprising. Indeed, our starting point, Eq. (1), is very close to a form one would have obtained by taking the expectation value of a two-body Hamiltonian. In the case of an energy functional calculated as the expectation value of a genuine Hamiltonian operator, the energy can be written not only as a functional of one-body transition densities, but also as a functional of projected one- and two-body (and eventually higher-order) densities. This freedom is lost in the functional framework, where a choice has to be made for either one or the other. MR-EDF follows the former strategy, whereas the latter has not been explored yet. For a regularized bilinear functional, the differences between both formulations remain very small, see Fig. 2.

(ii) Expression (19) contains not only one-body but also two-body matrix elements and might appear out of the scope of a density functional approach aiming at replacing the original N-body problem by a functional of the one-body density matrix only. Indeed, in the Hamiltonian case, the expectation value of any two-body Hamiltonian for any state can directly be regarded as a functional of the one- and two-body densities of this state. Density functional theories are introduced to avoid the explicit use of two-body and higher density matrices. Therefore, by itself, the use of a functional of the two-body density might appear useless. The important simplification here stems from the fact that these densities are constructed from a very specific class of states, namely, projected product states. For instance, we have shown recently that the two-body density matrix elements can eventually be written as an explicit functional of the one-body density under some approximation [14]. Accordingly, while two-body density matrix elements are used to get a compact expression in Eq. (19), this functional can truly be considered as a functional of the projected state one-body density consistently with density matrix functional theory, such that the sequence becomes

$$\Psi_N \Longrightarrow \rho^N \Longrightarrow \mathcal{E}_N\,. \tag{22}$$

(iii) When making the replacement (20) in Eq. (19), then the functional directly incorporates symmetry breaking and its restoration in a single step, contrary to standard approaches in EDF theory. From that point of view, it could be seen as a "symmetry-conserving" EDF theory.[4]

(iv) It is quite interesting to note that the MR-EDF can already almost be regarded as a functional of the components of the projected state. While this was hidden in formula (10), it becomes evident in Eq. (19). In particular, as noted in Refs. [6,8,11], there exists some flexibility in the regularization of the pathologies of the MR-EDF. It is possible to slightly modify the original prescription Eqs. (A4) and (A5), such that the regularization automatically leads to Eq. (20). In that case, the methods based on the use of MR-EDF and symmetry-conserved EDF framework are strictly equivalent. As an important consequence, while the use of techniques inspired from configuration mixing was unclear within a functional framework, we give here evidence that it can be formulated consistently in a functional framework. It is worth mentioning, however, that while this connection can be made only in the simple functional form given in Eq. (1), most functionals currently used do not allow their controlled usage in a MR-EDF framework.

(v) Finally, it is important to mention that this equivalence holds true only for the schematic bilinear functional given by Eq. (1) with two-body vertices independent of the density. If density-dependent terms are present in the functional, as in all currently used parametrizations of the EDF, such an equivalence does not exist anymore. Note, however, that in this case, a safely usable MR-EDF cannot be constructed anymore due to the absence of a regularization scheme. In Eq. (19), one then obtains a functional that remains closer to the spirit of DFT based on the Hohenberg-Kohn theorem than the usual MR-EDF approach. Indeed, in the HK-theorem-based DFT, the functional is constructed from the density matrices of the correlated (i.e., in our case projected) state. As we will illustrate below, on the contrary, the alternative formulation proposed here that simultaneously treats both symmetry breaking

[4]It should bekept in mind, however, that the present functional only takes care of the restoration of U(1) gauge symmetry while others still remain broken.

and restoration can still be applied for functionals that cannot be regularized in a MR-EDF framework.

A. Constraints on the symmetry-conserving functional

If the standard projection method is used as guidance to constructing the functional, then the form of the functional is almost entirely constrained. Indeed, this corresponds to using Eq. (13) or eventually Eq. (19) as a starting point. Equation (20) corresponds to a specific choice. Here, we discuss whether alternative choices can be made for the last two lines of Eq. (19). At present, it is not clear if, within the functional framework, a unique prescription of the functional form exists. Nevertheless, one can propose a few rules to better constrain its form. Let us assume a more general prescription than Eq. (20). i.e.,

$$\begin{aligned} \left(n_i^N n_i^N - \delta n_i \delta n_i\right) &\Longrightarrow F_{i\bar{i}}^N, \\ \left(n_i^N \left(1 - n_i^N\right) + \delta n_i \delta n_i\right) &\Longrightarrow G_{i\bar{i}}^N, \end{aligned} \tag{23}$$

where F^N and G^N are the unknown quantities. Let us specify some rules to constrain them:

Sum-rule. When $\overline{v}^{\rho\rho} = \overline{v}^{\kappa\kappa}$, then the last two terms in Eq. (13) should recombine to give $R_{i\bar{i}i\bar{i}}^N = n_i^N$. Accordingly, it seems reasonable to impose

$$F_{i\bar{i}}^N + G_{i\bar{i}}^N = n_i^N. \tag{24}$$

No-pairing limit. Slater determinants belong to the Hilbert space spanned by projected states. Consequently, one can interpret the functional for particle number projected wave functions as a generalization of the SR-EDF theory expressed for Slater determinant, i.e.,

$$\mathcal{E}_N[\Psi_N] \Longrightarrow \mathcal{E}_{\mathrm{SR}}[\Phi_{\mathrm{SD}}], \tag{25}$$

as $\Phi_N \longrightarrow \Phi_{\mathrm{SD}}$. Φ_{SD} denotes any Slater determinant. As a consequence, in this limit, we should have

$$F_{i\bar{i}}^N \Longrightarrow n_i^0 n_i^0, \quad G_{i\bar{i}}^N \Longrightarrow 0. \tag{26}$$

Large N limit. In the limit of infinite particle number, the projected state and the reference state should become identical (for instance, $\delta n_i^0 \Longrightarrow 0$). Accordingly, we do expect

$$\begin{aligned} \lim_{N\to+\infty} F_{i\bar{i}}^N &= n_i^N n_i^N, \\ \lim_{N\to+\infty} G_{i\bar{i}}^N &= n_i^N \left(1 - n_i^N\right). \end{aligned} \tag{27}$$

These three constraints significantly reduce the freedom of choosing the form of the functional that can be used. The prescription (20) naturally fulfills all of them.

B. Can we use terms with noninteger power of the density?

When the effective two-body vertex depends explicitly on the density, then the energy cannot be directly mapped on Eq. (13). If the density dependence is in integer powers of the density, then one could eventually generalize the derivation of Eq. (13) to three-body or even higher-order effective interactions. For all other forms of the density dependence, such as the widely used noninteger powers of the density,

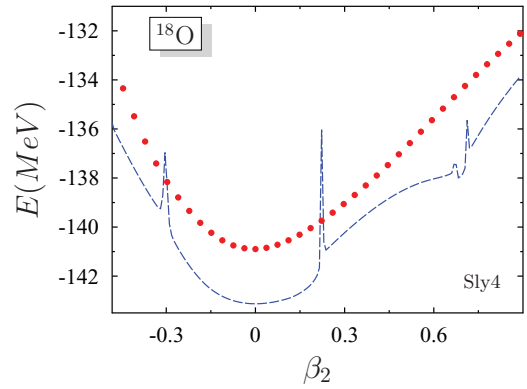

FIG. 3. (Color online) Same as Fig. 1, but when the SLy4 effective interaction is used in the particle-hole channel. The dashed line corresponds to the nonregularized MR-EDF result directly obtained by gauge angle integration using 199 points in the discretization. The filled circles correspond to the result obtained using the symmetry-conserved EDF using Eq. (19) and the prescription (20).

there is no way to deduce an equivalent expression because the integration over gauge angles cannot be uniquely defined from a mathematical point of view [5,11]. It is worth mentioning that the same difficulty appears when the Coulomb exchange term is approximated using the Slater prescription. Above, we have shown that with a slight change in the functional used in the standard MR-EDF method, one obtains an EDF that can be interpreted consistently within the usual functional approach where the projected state becomes a trial wave function to construct the ingredients of the functional.

Guided by the setup of functional (13), the most natural and simple way to extend the SR-EDF functional using density-dependent two-body effective vertices with noninteger powers of the density is to directly replace the density entering in the effective vertex by the density of the projected state, i.e.,

$$\overline{v}^{\rho\rho}[\rho] \Longrightarrow \overline{v}^{\rho\rho}[\rho^N], \quad \overline{v}^{\kappa\kappa}[\rho] \Longrightarrow \overline{v}^{\kappa\kappa}[\rho^N]. \tag{28}$$

Again, by doing this, we ensure that the functional used for the projected state is consistent with the one used in the no-pairing case Eq. (25) and in the large-N limit.

In Fig. 3, the deformation energy curve obtained by using Eq. (28) is compared to the result deduced from the standard nonregularized MR-EDF procedure using Eq. (10). The SLy4 effective interaction used here contains density-dependent terms with noninteger powers, i.e., $\rho^{2+1/6}$. Note that in this case, the MR-EDF cannot be regularized. The new alternative method we propose here, however, does lead to a perfectly well-behaved energy curve.

In our approach, the main difference between effective interactions that depend on noninteger powers of the density and those depending only on integer powers of the density is that while in the latter case one might eventually recognize terms coming from three-body or four-body forces and so on, this is impossible in the former case. It should, however, be kept in mind that the use of effective interactions should be regarded more as a guidance for the setup of the actual form of the functional and not as a prerequisite for the functional approaches as such.

The example of noninteger powers of the density shows that functional theory including pairing and particle number restoration and extending the usual SR-EDF approach, but without using the MR-EDF framework, can eventually be defined for a rather general class of functionals if the strategy to construct the functional proposed here is followed.

It is important to realize that for particle number projection, the present strategy becomes equivalent to the MR-EDF one when the regularization is slightly modified compared to the one originally proposed in Ref. [6], i.e., the present strategy and the modified regularized MR-EDF calculation will give the same energy for regularizable functionals. For those, it should therefore be more regarded as an alternative way of implementing the MR-EDF approach to particle number projection than as a new framework.

With the present strategy, one will never have practical difficulties in applying the method to rather general and complex forms of functionals. However, some effort has been made recently to outline the constraints that a functional should fulfill to be truly regarded as a symmetry-conserving functional [7]. While these constraints are even partially unknown, one might anticipate that they will significantly restrict the functional form that might be used. We are therefore facing the following dilemma: from condensed matter physics, we know that the powerfulness of DFT comes from the large flexibility in choosing the functional form. Putting too many formal constraints will make it increasingly difficult to model the relevant physics with a tractable functional. In particular, one can already see from Ref. [7] that a functional that fulfills the constraints elaborated there will be very close to the energy functional one obtains from an Hamiltonian.

It should also be mentioned that the use of the projected density entering effective density-dependent vertices $\bar{v}[\rho^N]$ has already been proposed and used in Refs. [15–17]. However, in those references, a hybrid approach is set up where transition densities are used in other parts of the functional, and for the restoration of spatial symmetries.[5] It has been pointed out in Ref. [13] that such a hybrid approach may lead to unphysical results when set up for the restoration of spatial symmetries. Here, the theory is completely formulated in terms of the projected one- and two-body density matrices only. An open question that has to be addressed in the future is if and how the strategy to set up the functional we propose here can be generalized to the restoration of spatial symmetries, and perhaps even more general configuration mixing without becoming numerically intractable.

IV. DISCUSSION AND CONCLUSION

In this work, projection made by MR-EDF techniques including the recently proposed regularization [6,8,11] is further analyzed for the case of particle number restoration of quasi-particle vacua of Bogoliubov type. Starting from a simple toy functional where the two-body effective interaction is not explicitly density dependent, we show that the regularized energy can *almost* be regarded as a functional of the one- and two-body densities of the projected state. To follow the density functional methodology, we propose to slightly modify the functional such that it becomes a function of projected state densities *only*, and that the projected state becomes the intermediate trial state from which the functional and other observables are constructed. For particle number projection, such a modification could, for instance, be achieved within standard MR-EDF theory by slightly modifying the regularization proposed in Ref. [6] while still removing the pathologies. Such an alternative interpretation may eventually serve as a justification of the MR-EDF framework within a functional approach for particle number restoration when the effective kernels are not density dependent.

As a matter of fact, most of the functional forms used nowadays do not enter into the class of functionals which can be safely used in MR-EDF. We show, however, that such a functional can still be used in a symmetry restoring framework that does not make use of the MR-EDF technique, but directly formulates the theory in terms of the one- and two-body density matrices of projected product states.

This theory can be seen as a direct extension of the SR-EDF level that we proposed and is called here the symmetry-conserving EDF approach. An illustration of the resulting projected energy is given, showing that the method could be a valuable tool for the description of the ground state of a system with pairing including the restoration of particle number even when density dependence with noninteger powers is used in the functional.

The analysis of similarities and differences between the MR-EDF theory and symmetry-conserving approaches was greatly simplified here because the original quasi-particle state and the projected state share the same canonical basis. For instance, expression (19) only holds in the canonical basis. In the present article, the applications are restricted to projection after variation for which this equation is perfectly suited. The next step will be the extension approach to perform variation after projection (VAP). VAP is usually solved using MR-EDF techniques by making variations with respect to the components of the original quasi-particle vacuum and not the projected state itself [20–23]. In the symmetry-conserving approach, one could follow the same strategy as in the standard MR-EDF approach, i.e., perform variations of the reference state. Work in that direction is currently underway.

Last, we would like to mention that the present article only discusses the case of particle number projection and the possibility to determine the ground-state energy. The MR-EDF technique is frequently used to restore other symmetries and to calculate excited states in a generator-coordinate framework. What these other configuration mixings have in common is the fact that there does not exist a common canonical basis in which the one-body density matrices of the original and of the correlated states are simultaneously diagonal. An important point to be clarified is if and how the formalism developed here can be generalized to those more general configuration mixings, and that without becoming numerically intractable.

[5]For the special case of a pure particle number projected MR-EDF calculation, the functional used in Refs. [17–19] could be mapped on a functional of the one- and two-body density matrices of the projected state.

Finally, it has to be stressed that the method proposed and explored here is not meant to replace the MR-EDF framework for the description of excited states and transition moments in complex nuclei. Instead, it might provide a numerically much more efficient alternative to the MR-EDF scheme when one is interested just in the ground state and its evolution, either in dynamics or thermodynamics.

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APPENDIX A: PROOF OF Eq. (19)

To prove Eq. (19), we have to explicitly remove terms that cause pathologies from the energy calculation as proposed in Ref. [6]. Starting from Eq. (50) of Ref. [6], the transition matrix elements can be expressed as

$$\begin{aligned} n_i^{0\varphi} &\equiv n_i^0 + \delta n_i\,[\varphi]\,, \\ \kappa_{i\bar{i}}^{0\varphi} &\equiv \kappa_{i\bar{i}}^0 + \delta\kappa_{i\bar{i}}\,[\varphi]\,, \\ \kappa_{i\bar{i}}^{\varphi 0\star} &\equiv \kappa_{i\bar{i}}^{0*} + \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,, \end{aligned} \tag{A1}$$

where n_i^0 and $\kappa_{i\bar{i}}^0$ refer to the occupation probabilities and anomalous densities of the state Φ_0. Following Ref. [6], we decompose the energy kernels entering into the integral of Eq. (10) into three terms $\mathcal{E}^{\rho}$, $\mathcal{E}^{\rho\rho}$, and $\mathcal{E}^{\kappa\kappa}$ corresponding to the kinetic, mean-field, and pairing terms, respectively. Then, $\mathcal{E}^{\rho\rho}$ and $\mathcal{E}^{\kappa\kappa}$ can be expressed as

$$\begin{aligned} \mathcal{E}^{\rho\rho} = &\frac{1}{2}\sum_{ij}\bar{v}_{ijij}^{\rho\rho} n_i^0 n_j^0 + \frac{1}{2}\sum_{ij}\bar{v}_{ijij}^{\rho\rho}\left(n_i^0\delta n_j\,[\varphi] + n_j^0\delta n_i\,[\varphi]\right) \\ &+ \frac{1}{2}\sum_{ij}\bar{v}_{ijij}^{\rho\rho}\delta n_i\,[\varphi]\,\delta n_j\,[\varphi]\,, \end{aligned} \tag{A2}$$

whereas

$$\begin{aligned} \mathcal{E}^{\kappa\kappa} = &\frac{1}{4}\sum_{ij}\bar{v}_{i\bar{i}j\bar{j}}^{\kappa\kappa}\kappa_{i\bar{i}}^{0*}\kappa_{j\bar{j}}^0 \\ &+ \frac{1}{4}\sum_{ij}\bar{v}_{i\bar{i}j\bar{j}}^{\kappa\kappa}\left(\kappa_{i\bar{i}}^{0*}\delta\kappa_{j\bar{j}}\,[\varphi] + \kappa_{j\bar{j}}^0\delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\right) \\ &+ \frac{1}{4}\sum_{ij}\bar{v}_{i\bar{i}j\bar{j}}^{\kappa\kappa}\delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,\delta\kappa_{j\bar{j}}\,[\varphi]\,. \end{aligned} \tag{A3}$$

These expressions are the strict equivalent of the ones given in Eqs. (51)–(54) in Ref. [6]. For instance, regularizations have been obtained by removing terms with $j = \bar{i}$ in the last line of Eqs. (A2) and (A3). Accordingly, the spurious contribution to be removed from the functional is

$$\mathcal{E}_{\mathrm{CG}}^{\rho\rho} = \frac{1}{2}\sum_i \bar{v}_{ijij}^{\rho\rho}\int \delta n_i\,[\varphi]\,\delta n_i\,[\varphi]\,\mathcal{N}_N(0,\varphi)d\varphi\,, \tag{A4}$$

$$\mathcal{E}_{\mathrm{CG}}^{\kappa\kappa} = \frac{1}{2}\sum_i \bar{v}_{iiii}^{\kappa\kappa}\int \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,\delta\kappa_{i\bar{i}}\,[\varphi]\,\mathcal{N}_N(0,\varphi)d\varphi\,. \tag{A5}$$

Therefore, when the regularization is included, this is equivalent to making the replacements

$$\begin{aligned} &\int_0^{2\pi} d\varphi n_i^{0\varphi} n_i^{0\varphi}\mathcal{N}_N(0,\varphi) \\ &\quad\Longrightarrow \int_0^{2\pi} d\varphi\left(n_i^{0\varphi} n_i^{0\varphi} - \delta n_i\,[\varphi]\,\delta n_i\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \end{aligned}$$

and

$$\begin{aligned} &\int_0^{2\pi} d\varphi\kappa_{i\bar{i}}^{\varphi 0\star}\kappa_{i\bar{i}}^{0\varphi}\mathcal{N}_N(0,\varphi) \\ &\quad\Longrightarrow \int_0^{2\pi} d\varphi\left(\kappa_{i\bar{i}}^{\varphi 0\star}\kappa_{i\bar{i}}^{0\varphi} - \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,\delta\kappa_{i\bar{i}}\,[\varphi]\right)\mathcal{N}_N(0,\varphi)\,, \end{aligned}$$

in the last two terms of Eq. (13).

From the equalities (A1), one can deduce new interesting relationships between the projected observables. For instance, performing the gauge integration of the first equation, we obtain

$$n_i^N = \int_0^{2\pi} d\varphi n_i^{0\varphi}\mathcal{N}_N(0,\varphi) = n_i^0 + \delta n_i\,, \tag{A6}$$

with

$$\delta n_i = n_i^N - n_i^0 = \int d\varphi\,\delta n_i\,[\varphi]\,\mathcal{N}_N(0,\varphi)\,. \tag{A7}$$

From this, let us now re-express the different quantities entering in Eq. (13)

$$\begin{aligned} &\int_0^{2\pi} d\varphi n_i^{0\varphi} n_j^{0\varphi}\mathcal{N}_N(0,\varphi) \\ &= n_i^0 n_j^0 + n_i^0\delta n_j + \delta n_i n_j^0 + \int_0^{2\pi} d\varphi\delta n_i\,[\varphi]\,\delta n_j\,[\varphi]\,\mathcal{N}_N(0,\varphi)\,, \end{aligned}$$

where, in the specific case $i = j$, we recognize the term that enters in the regularization to be the last one. Therefore, the term entering into the regularization of $\mathcal{E}^{\rho\rho}$ can be expressed as

$$\begin{aligned} &\int_0^{2\pi} d\varphi\left(n_i^{0\varphi} n_i^{0\varphi} - \delta n_i\,[\varphi]\,\delta n_i\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \\ &\quad = n_i^0 n_i^0 + 2n_i^0\delta n_i = n_i^N n_i^N - \delta n_i\delta n_i\,. \end{aligned} \tag{A8}$$

To derive an expression of the term entering in the regularization of $\mathcal{E}^{\kappa\kappa}$, one can proceed in a similar way. We first define $\delta\kappa_{i\bar{i}}^*$ and $\delta\kappa_{i\bar{i}}$ through

$$\begin{aligned} \int_0^{2\pi} d\varphi\kappa_{i\bar{i}}^{\varphi 0\star}\mathcal{N}_N(0,\varphi) &= \int_0^{2\pi} d\varphi\left(\kappa_{i\bar{i}}^{0*} + \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \\ &\equiv \kappa_{i\bar{i}}^{0*} + \delta\kappa_{i\bar{i}}^{\star}\,, \\ \int_0^{2\pi} d\varphi\kappa_{i\bar{i}}^{0\varphi}\mathcal{N}_N(0,\varphi) &= \int_0^{2\pi} d\varphi\left(\kappa_{i\bar{i}}^{0} + \delta\kappa_{i\bar{i}}\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \\ &\equiv \kappa_{i\bar{i}}^{0} + \delta\kappa_{i\bar{i}}\,. \end{aligned}$$

Therefore the term entering in the regularized functional is given by

$$\begin{aligned} &\int_0^{2\pi} d\varphi\left(\kappa_{i\bar{i}}^{\varphi 0\star}\kappa_{i\bar{i}}^{0\varphi} - \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,\delta\kappa_{i\bar{i}}\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \\ &\quad = \kappa_{i\bar{i}}^{0*}\kappa_{i\bar{i}}^0 + \delta\kappa_{i\bar{i}}^{\star}\kappa_{i\bar{i}}^0 + \kappa_{i\bar{i}}^{0*}\delta\kappa_{i\bar{i}}\,. \end{aligned} \tag{A9}$$

One can then take advantage of the fact that

$$\begin{aligned} n_i^N &= n_i^0 n_i^0 + 2n_i^0 \delta n_i \\ &+ \int_0^{2\pi} d\varphi \delta n_i\,[\varphi]\,\delta n_j\,[\varphi]\,\mathcal{N}_N(0,\varphi) \\ &+ \kappa_{i\bar{i}}^{0*}\kappa_{i\bar{i}}^{0} + \delta\kappa_{i\bar{i}}^{\star}\kappa_{i\bar{i}}^{0} + \kappa_{i\bar{i}}^{0*}\delta\kappa_{i\bar{i}} \\ &+ \int_0^{2\pi} d\varphi \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,\delta\kappa_{i\bar{i}}\,[\varphi]\,\mathcal{N}_N(0,\varphi), \end{aligned}$$

and that

$$\delta n_i\,[\varphi]\,\delta n_i\,[\varphi] = -\delta\kappa_{i\bar{i}}\,[\varphi]\,\delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,. \tag{A10}$$

The first equality is nothing but Eq. (18), whereas the second equality can be proved by expressing $\delta n_i\,[\varphi]$, $\delta\kappa_{i\bar{i}}\,[\varphi]$, and $\delta\kappa_{i\bar{i}}^{*}\,[\varphi]$ directly in terms of the u_i and v_i of the SR-EDF theory and the gauge angle φ starting from Eqs. (72)–(74) of Ref. [6]. Altogether, we obtain

$$\begin{aligned} &\int_0^{2\pi} d\varphi \left(\kappa_{i\bar{i}}^{\varphi 0\star}\kappa_{i\bar{i}}^{0\varphi} - \delta\kappa_{i\bar{i}}^{\star}\,[\varphi]\,\delta\kappa_{i\bar{i}}\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \\ &\quad = n_i^N - \int_0^{2\pi} d\varphi \left(n_i^{0\varphi} n_i^{0\varphi} - \delta n_i\,[\varphi]\,\delta n_i\,[\varphi]\right)\mathcal{N}_N(0,\varphi) \\ &\quad = \left(n_i^N\left(1-n_i^N\right) + \delta n_i \delta n_i\right). \end{aligned} \tag{A11}$$

Combining this expression with Eq. (A8), we finally deduce the expression (19) for the regularized functional.

APPENDIX B: PARTICLE NUMBER RESTORATION WITH RECURRENCE RELATION

An alternative to the the gauge-integration method is presented here to calculate the one- and two-body density matrix components of a projected product state. This method turns out to be very fast and efficient numerically.

Let us start from a quasi-particle state written in its canonical basis as

$$|\Phi_0\rangle = \prod_{i>0}(1 + x_i a_i^{\dagger} a_{\bar{i}}^{\dagger})|0\rangle\,, \tag{B1}$$

where $|x_i|^2 = n_i^0/(1-n_i^0)$. The associated projected state with N particles can be expressed as

$$|\Psi_N\rangle \propto \left(\sum_{i>0} x_i a_i^{\dagger} a_{\bar{i}}^{\dagger}\right)^N |0\rangle\,. \tag{B2}$$

Starting from these expressions, it has recently been shown [14] that the elements of the one- and two-body density matrix are given by

$$n_i^N = N|x_i|^2 \frac{I_{N-1}(i)}{I_N}\,, \tag{B3}$$

$$R_{i\bar{i}j\bar{j}}^N = N x_i^* x_j \frac{I_{N-1}(i,j)}{I_N} \quad \text{for} \quad (i \neq j)\,, \tag{B4}$$

$$R_{ijij}^N = N(N-1)|x_i|^2|x_j|^2 \frac{I_{N-2}(i,j)}{I_N}\,, \tag{B5}$$

while as already mentioned, $R_{i\bar{i}i\bar{i}}^N = n_i^N$. The different coefficients entering in n^N and R^N are given by

$$\begin{aligned} I_K &= \sum_{(i_1,\ldots,i_K)}^{\neq} |x_{i_1}|^2 \cdots |x_{i_K}|^2, \\ I_K(i) &= \sum_{(i_1,\ldots,i_K)\neq i}^{\neq} |x_{i_1}|^2 \cdots |x_{i_K}|^2, \\ I_K(i,j) &= \sum_{(i_1,\ldots,i_K)\neq (i,j)}^{\neq} |x_{i_1}|^2 \cdots |x_{i_K}|^2, \\ &\cdots \end{aligned}$$

Direct use of these expressions for $K = N$ is rather difficult numerically. However, these coefficients verify simple recurrence relations that are straightforward to implement on a computer. These recurrence relations have been recently used to solve numerically the VAP [24,25] and to set up a new functional for pairing accounting for particle number conservation [14].

In the present work, we use the recurrence method to perform PAV within the symmetry-conserving EDF framework. In that case, a preliminary SR-EDF calculation is performed leading to a quasi-particle state given by Eq. (B1) with a set of $\{x_i\}$ values. Here, we have used the Ev8 code [26]. From this set, the quantities $I_{N-1}(i)$ and I_N are evaluated via the recurrence relations

$$\begin{aligned} I_K(i) &= I_K - (K-1)|x_i|^2 I_{K-1}(i), \\ I_K &= \sum_i |x_i|^2 I_{K-1} - (K-2)\sum_i |x_i|^4 I_{K-2}(i)\,, \end{aligned} \tag{B6}$$

with the condition $I_0 = I_0(i) = 1$, $I_1 = \sum_k |x_k|^2$, and $I_1(i) = I_1 - |x_i|^2$. The occupation numbers of the projected state can then be calculated as well as the correlation components using the relation [14,27]

$$R_{i\bar{i}j\bar{j}}^N = x_i^* x_j \frac{n_j^N - n_i^N}{|x_j|^2 - |x_i|^2} \quad \text{for} \quad (i \neq j), \tag{B7}$$

$$R_{ijij}^N = \frac{|x_j|^2 n_i^N - |x_i|^2 n_j^N}{|x_j|^2 - |x_i|^2}\,, \tag{B8}$$

where for $i = j$, we have $R_{i\bar{i}j\bar{j}}^N = n_i^N$ and $R_{ijij}^N = 0$. This method is referred to as the recurrence method in the text.

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