On the formulation of functional theory for pairing with particle number restoration

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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 non-projected 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 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, 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, like 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 where 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 non-regularized nor the regularized functionals can straightforwardly be interpreted in terms of the densities of projected or non-projected 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 non-analytical density dependences.

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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. At the so-called Single-Reference (SR) level, a quasi-particle (QP) vacuum of Bogoliubov type |Φ₀⟩ 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

\[ E_{SR}[Φ₀] = E_{SR}[ρ, κ, κ^*] = \sum_i t_i ρ_{ii} + \frac{1}{2} \sum_{i,j} τ_{ij}^ρ ρ_{ii} ρ_{jj} + \frac{1}{4} \sum_{i,j} τ_{ij}^{κκ} κ_{ii}^* κ_{jj}, \]  

where τ^ρ and τ^{κκ} denote the effective vertices in the particle-hole and particle-particle channels. Standard SR-EDF can be schematically seen as the sequence

|Φ₀⟩ \Rightarrow (ρ, κ, κ^*) \Rightarrow E_{SR}. \tag{2} \]

The price to be paid for incorporating pairing with a rather simple functional is to use an intermediate state |Φ₀⟩ that is not an eigenstate of particle number. In a second step, the symmetry can be restored projecting out the component with N particles

|Ψ_N⟩ = P_N |Φ₀⟩, \tag{3} \]

where P_N denotes the particle number projection operator defined through [2, 3]

\[ P_N = \frac{1}{2} \int_{0}^{2π} dφ e^{iφ(\hat{N}−N)} . \tag{4} \]

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

\[ \langle Ψ_N | O | Ψ_N \rangle \rightarrow \int_{0}^{2π} dφ \frac{⟨Φ₀ | O | Φ_φ⟩ }{ ⟨Φ₀ | Φ_φ⟩ } N_N(0, φ) , \tag{5} \]

where the shorthand

\[ N_N(0, φ) \equiv \frac{e^{−iφ\hat{N}} ⟨Φ₀ | Φ_φ⟩ }{ 2π ⟨Ψ_N | Ψ_N⟩ } . \tag{6} \]

has been introduced. Here φ denotes the gauge angle, whereas |Φ_φ⟩ = e^{iφ\hat{N}} |Φ₀⟩ refers to the state |Φ₀⟩ 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 Theorem (GWT) [2, 12] to express the kernel in terms of the transition density matrices

\[ ρ_{ij}^{0φ} = \frac{⟨Φ₀ | a_j^† a_i | Φ_φ⟩ }{ ⟨Φ₀ | Φ_φ⟩ } , \tag{7} \]

\[ κ_{ij}^{φ} = \frac{⟨Φ₀ | a_j a_i | Φ_φ⟩ }{ ⟨Φ₀ | Φ_φ⟩ } , \tag{8} \]

\[ κ^{φ0*} = \frac{⟨Φ₀ | a_j^† a_i | Φ_φ⟩ }{ ⟨Φ₀ | Φ_φ⟩ } . \tag{9} \]

For instance, when O is a two-body Hamiltonian, the two-body interaction \( τ \) entering in (5) takes a form similar to Eq. (1) with \( τ^{ρρ} = τ^{κκ} = τ \) 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

\[ E_N[Ψ_N] = \int_{0}^{2π} dφ E_{SR} \left[ ρ_{ij}^{0φ}, κ_{ij}^{φ}, κ^{φ0 *} \right] N_N(0, φ) . \tag{10} \]

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:

- The expression (10) is postulated having in mind the Hamiltonian case. However, the MR-EDF theory should not be confused 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.
- 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 non-integer 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 basis 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

$$
\rho_{ij}^0 = \delta_{ij} n_i^0, \quad \rho_{ij}^{0\varphi} = \delta_{ij} n_i^{0\varphi}, \quad \kappa_{ij}^{0\varphi*} = \delta_{ij} \kappa_{ii}^{0\varphi*},
$$

whereas the energy $E_N$ takes the form

$$
E_N[\Psi_N] = \sum_i t_{ii} n_i^0 N_N(0, \varphi)
+ \frac{1}{2} \sum_{i,j} \varpi_{ij|ii}^0 n_i^0 n_j^0 N_N(0, \varphi)
+ \frac{1}{4} \sum_{i,j} \varpi_{ij|ii}^{0\varphi*} \kappa_{ij}^{0\varphi*} N_N(0, \varphi),
$$

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

$$
E_N[\Psi_N] = \sum_i t_{ii} n_i^N
+ \frac{1}{2} \sum_{i,j \neq i} \varpi_{ij|ii}^{0\varphi} R_{ij|ii}^N
+ \frac{1}{4} \sum_{i \neq j, i \neq \bar{i}} \varpi_{ij|ii}^{0\varphi*} R_{ii|ij}^N
+ \frac{1}{2} \sum_i \varpi_{ii|ii}^{0\varphi} \int d\varphi n_i^0 n_i^0 N_N(0, \varphi)
+ \frac{1}{2} \sum_i \varpi_{ii|ii}^{0\varphi*} \int d\varphi \kappa_{ii}^{0\varphi*} \kappa_{ii}^{0\varphi*} N_N(0, \varphi),
$$

where $n_i^N$ are the occupation numbers:

$$
n_i^N = \frac{\langle \Psi_N | a_i^\dagger a_i | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle}
$$

and $R_{ii|ij}^N$ corresponds to the two-body density matrix

$$
R_{ii|ij}^N = \frac{\langle \Psi_N | a_i^\dagger a_j^\dagger a_i a_j | \Psi_N \rangle}{\langle \Psi_N | \Psi_N \rangle}
$$

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

$$
n_i^N = \int_0^{2\pi} d\varphi \ n_i^{0\varphi} N_N(0, \varphi),
$$

and

$$
R_{ij|ii}^N = \int_0^{2\pi} d\varphi \ n_i^{0\varphi} n_j^{0\varphi} N_N(0, \varphi)
= \int_0^{2\pi} d\varphi \ n_i^{0\varphi} n_j^{0\varphi} N_N(0, \varphi)
= \int_0^{2\pi} d\varphi \ n_i^{0\varphi} n_j^{0\varphi} N_N(0, \varphi).
$$

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 $\varpi^{0\varphi} = \varpi^{0\varphi}$, then the last two terms of Eq. (13) recombine and the two-body component $R_{ii|ii}^N$ can be recognized, thanks to the relation

$$
R_{ii|ii}^N = n_i^N
= \int_0^{2\pi} d\varphi \ (n_i^{0\varphi} n_i^{0\varphi} + \kappa_{ii}^{0\varphi*} \kappa_{ii}^{0\varphi*}) N_N(0, \varphi).
$$

However, when using different effective vertices $\varpi^{0\varphi} \neq \varpi^{0\varphi}$ in the particle-hole and particle-particle channels, or when using vertices $\varpi^{0\varphi}$ or $\varpi^{0\varphi}$ 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 $\langle \Phi_0 | \Phi_\varphi \rangle \approx 0$ there is at least one $n_i^{0\varphi}$ and the corresponding $\kappa_{ii}^{0\varphi*}$ and $\kappa_{ii}^{0\varphi*}$ 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 $\varpi^{0\varphi} = \varpi^{0\varphi}$. 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.

$^2$ 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.
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)

$$\mathcal{E}_N[\Psi_N] = \sum_i t_i n_i^N + \frac{1}{2} \sum_{i,j \neq i} \tau_{ij}^p R_{ij}^{N} + \frac{1}{4} \sum_{i,j,j' \neq i} \tau_{ij}^{pp} p_{ij}^{N} + \frac{1}{2} \sum_i \left( \tau_{ii}^p (n_i^N - \delta n_i \delta n_i) \right. + \left. \frac{1}{2} \sum_i \tau_{ii}^{pp} \left[ n_i^1 (1 - n_i^N + \delta n_i \delta n_i) \right. \right), \quad (19)$$

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 non-projected 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 non-projected state. The analysis of the regularization procedure to remove spurious contribution to the MR-EDF method [6, 8, 11] suggests that these terms will always be well-behaved.

An example for 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 non-regularized MR-EDF [8]. As in Ref. [8], the Lipkin-Nogami procedure is used in the minimization of the energy of the state $|\Phi_0\rangle$. The solid line corresponds to the MR-EDF method with the regularization proposed in [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 "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 to be very simple, numerically efficient and to not make 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 non-analytical density dependence, for example a non-integer power such as often used in parameterizations 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 which density, i.e. projected, transition, or non-projected 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. DISCUSSION ON 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 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

\[
(n_i^N n_i^N - \delta n_i \delta n_i) \implies n_i^N n_i^N,
\]

\[
[n_i^N(1 - n_i^N) + \delta n_i \delta n_i] \implies n_i^N(1 - n_i^N),
\]

(20)

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

The use of a projected product state a auxiliary state has the advantage that it allows 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 \( \delta n_i \) (resp. \( \delta n_i \delta n_i \)) is likely to be much smaller than \( n_i^N \) (resp. \( n_i^N n_i^N \)).

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

\[
\Psi_N \implies (\rho^N, R^N) \implies \mathcal{E}_N.
\]

(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:

- 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 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.

- 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

\[^3\] 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.
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 become

\[
\Psi_N \implies \rho^N \implies \mathcal{E}_N. \tag{22}
\]

- 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

- 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 (A4-A5), such that the regularization automatically leads to (20). In that case, the method 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, however, worth mentioning 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 an MR EDF framework.

- Finally, it is important to mention that this equivalence holds only true for the schematic bilinear functional given by Eq. (1) with two-body vertices independent on the density. If density dependent terms are present in the functional, like in all currently used parameterizations 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 treats both symmetry breaking and restoration simultaneously 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 construct the functional, then the form of the functional is almost entirely constrained. Indeed, this corresponds to use Eq. (13) or eventually Eq. (19) as a starting point. Eq. (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)

\[
(n_i^N n_i^N - \delta n_i \delta n_i) \implies F_{ii}^N, \tag{23}
\]

\[
(n_i^N (1 - n_i^N) + \delta n_i \delta n_i) \implies G_{ii}^N,
\]

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

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

\[
F_{ii}^N + G_{ii}^N = n_i^N. \tag{24}
\]

- **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.

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

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

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

\[ F_{ii}^N \mapsto n_i^N n_i^0, \quad G_{ii}^N \mapsto 0. \tag{26} \]

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

\[ \lim_{N \to \infty} F_{ii}^N = n_i^N n_i^N, \]
\[ \lim_{N \to \infty} G_{ii}^N = n_i^N (1 - n_i^N). \tag{27} \]

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 non integer 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 non-integer powers of the density, 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 to mention 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 obtain 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 non-integer powers of the density is to directly replace the density entering in the effective vertex by the density of the projected state, i.e.

\[ \varphi^{(p)}[\rho] \mapsto \varphi^{(p)}[\rho^N], \quad \varphi^{(k)}[\rho] \mapsto \varphi^{(k)}[\rho^N]. \tag{28} \]

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 non-regularized MR-EDF procedure using Eq. (10). The SLy4 effective interaction used here contains density dependent terms with non-integer 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 non-integer 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 set-up of the actual form of the functional, and not as a prerequisite for the functional approaches as such.

The example of non-integer 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 rather general class of functionals if the strategy to construct the functional proposed here is followed. Let us add a few remarks:

- 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 MR-EDF approach to particle-number projection than as a new framework.
- With the present strategy, one will never have prac-
tical difficulties in applying the method to rather
general and complex forms of functionals. How-
ever, some effort has been made recently to out-
line the constraints that a functional should ful-
fill 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 fol-
lowing 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 ful-
fills the constraints elaborated there will be very
close to the energy functional one obtains from an
Hamiltonian.

- It should be mentioned that the use of the pro-
jecteded density entering effective density-dependent
vertices $v(\rho^n)$ has already been proposed and used
in Refs. [15–17]. However, in those references, a hy-
brid approach is set up where transition densities
are used in other parts of the functional, and for
the restoration of spatial symmetries. It has been
pointed out in Ref. [13] that such 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 resto-
ration of spatial symmetries, and perhaps even more
general configuration mixing without becoming nu-
merically 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 resto-
ration of quasi-particle vacua of Bogoliubov type. Starting
from a simple toy functional where the two-body effec-
tive 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 method-
ology, 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 inter-
mediate trial state from which the functional and other
observables are constructed. For particle-number projec-
tion, such a modification could for instance be achieved
within standard MR-EDF by slightly modifying the reg-
ularization proposed in Ref. [6] while still removing
the pathologies. Such an alternative interpretation may
eventually serve as a justification of MR-EDF framework
within a functional approach for particle number resto-
ration 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 functional can still be used in a symmetry restoring
framework that does not make use of the MR-EDF tech-
nique, 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 Symmetry-
Conserving EDF approach. An illustration of the result-
ing 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
non-integer 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 ap-
lications are restricted to projection after variation for
which this equation is perfectly suited. The next the 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 com-
ponents of the original quasi-particle vacuum and not the
projected state itself [20–23]. In the symmetry conserv-
ning 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 ar-
ticle only discusses the case of particle-number projec-
tion 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 im-
portant 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 nu-
merically intractable. Finally, it has to be stressed that

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

\[
\begin{align*}
\tilde{v}^{00}_{ij} &\equiv \tilde{v}^{00}_{ij} + \delta n_i [\varphi], \\
\kappa^{0*}_{ii} &\equiv \kappa^{0*}_{ii} + \delta \kappa_{ii} [\varphi] , \\
\kappa^0_{ii} &\equiv \kappa^0_{ii} + \delta \kappa^0_{ii} [\varphi],
\end{align*}
\]

where \( n_i^0 \) and \( \kappa^0_{ii} \) refer to the occupation probabilities and anomalous densities of the state \( \Phi_0 \). Following Ref. [6], we decompose the energy kernels entering into the integral of Eq. (eq:ekernel) into three terms \( \mathcal{E}^p, \mathcal{E}^{pp} \) and \( \mathcal{E}^{\kappa\kappa} \) corresponding to the kinetic, mean-field and pairing terms respectively. Then, \( \mathcal{E}^{pp} \) and \( \mathcal{E}^{\kappa\kappa} \) can be expressed as

\[
\begin{align*}
\mathcal{E}^{pp} &= \frac{1}{2} \sum_{ij} \tilde{v}^{pp}_{ijij} n_i^0 n_j^0 \\
&\quad + \frac{1}{2} \sum_{ij} \tilde{v}^{pp}_{ijij} \left( n_i^0 \delta n_j [\varphi] + n_j^0 \delta n_i [\varphi] \right) \\
&\quad + \frac{1}{2} \sum_{ij} \tilde{v}^{pp}_{ijij} \delta n_i [\varphi] \delta n_j [\varphi],
\end{align*}
\]

whereas

\[
\begin{align*}
\mathcal{E}^{\kappa\kappa} &= \frac{1}{4} \sum_{ij} \tilde{v}^{\kappa\kappa}_{ijij} \kappa^{0*}_{ii} \kappa^0_{jj} \\
&\quad + \frac{1}{4} \sum_{ij} \tilde{v}^{\kappa\kappa}_{ijij} \left( \kappa^{0*}_{ii} \delta \kappa_{jj} [\varphi] + \kappa^0_{jj} \delta \kappa^0_{ii} [\varphi] \right) \\
&\quad + \frac{1}{4} \sum_{ij} \tilde{v}^{\kappa\kappa}_{ijij} \delta \kappa_{ii} [\varphi] \delta \kappa_{jj} [\varphi].
\end{align*}
\]

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

\[
\begin{align*}
\mathcal{E}_{CG}^{pp} &= \frac{1}{2} \sum_{ij} \tilde{v}^{pp}_{ijij} \int \delta n_i [\varphi] \delta n_i [\varphi] \mathcal{N}_N(0, \varphi) d\varphi, \\
\mathcal{E}_{CG}^{\kappa\kappa} &= \frac{1}{2} \sum_{ij} \tilde{v}^{\kappa\kappa}_{ijij} \int \delta \kappa_i [\varphi] \delta \kappa_i [\varphi] \mathcal{N}_N(0, \varphi) d\varphi.
\end{align*}
\]

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

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

and

\[
\begin{align*}
\int_0^{2\pi} d\varphi \kappa_i^{0*} \kappa_j^{0*} \mathcal{N}_N(0, \varphi) \\
&\quad \int_0^{2\pi} d\varphi \left( \kappa_i^{0*} \kappa_j^{0*} - \delta \kappa_i [\varphi] \delta \kappa_j [\varphi] \right) \mathcal{N}_N(0, \varphi),
\end{align*}
\]

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

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

with

\[
\delta n_i = n_i^N - n_i^0 = \int_0^{2\pi} d\varphi \delta n_i [\varphi] \mathcal{N}_N(0, \varphi).
\]

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

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

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 \( \mathcal{E}^{pp} \) can be expressed as

\[
\begin{align*}
\int_0^{2\pi} d\varphi \left( n_i^{0\varphi} n_i^{0\varphi} - \delta n_i [\varphi] \delta n_i [\varphi] \right) \mathcal{N}_N(0, \varphi) \\
&\quad = n_i^0 n_i^0 + 2n_i^0 \delta n_i \\
&\quad = n_i^N n_i^N - \delta n_i \delta n_i.
\end{align*}
\]
To derive an expression of the term entering in the regularized of $\mathcal{E}^{\kappa\kappa}$, one can proceed in a similar way. We first define $\delta \kappa_{ii}^0$ and $\delta \kappa_{ij}$ through

$$\int_{0}^{2\pi} d\varphi \, \kappa_{ii}^{0*} N_{ii}(0, \varphi) = \int_{0}^{2\pi} d\varphi \left( \kappa_{ii}^{0*} + \delta \kappa_{ii}^* \right) N_{ii}(0, \varphi)$$

$$= \kappa_{ii}^{0*} + \delta \kappa_{ii}^* \equiv \kappa_{ii}^{0*} + \delta \kappa_{ii}^* .$$

Therefore the term entering in the regularized functional is given by

$$\int_{0}^{2\pi} d\varphi \left( \kappa_{ii}^{*0} \kappa_{ii}^{0} - \delta \kappa_{ii}^* \kappa_{ii}^* \right) N_{ii}(0, \varphi)$$

$$= \kappa_{ii}^{0*} \kappa_{ii}^{0} + \delta \kappa_{ii}^* \kappa_{ii}^* + \kappa_{ii}^{0} \delta \kappa_{ii}^* .$$

One can then take advantage of the fact that

$$n_i^N = n_i^0 n_i^0 + 2 n_i^0 n_i^1 +$$

$$+ \int_{0}^{2\pi} d\varphi \, \delta n_i [\varphi] \delta n_j [\varphi] N_{ii}(0, \varphi)$$

$$+ \kappa_{ii}^{0*} \kappa_{ii}^{0} + \delta \kappa_{ii}^* \kappa_{ii}^* + \kappa_{ii}^{0} \delta \kappa_{ii}^*$$

and that

$$\delta \kappa_{ii}^* \kappa_{ii}^* \equiv - \delta \kappa_{ii}^* \delta \kappa_{ii}^* .$$

The first equality is nothing but Eq. (18), whereas the second equality can be proved by expressing $\delta n_i [\varphi]$, $\delta \kappa_{ii}^* [\varphi]$ and $\kappa_{ii}^{0*} \kappa_{ii}^{0} \delta \kappa_{ii}^* \kappa_{ii}^*$ directly in terms of the $u_i$ and $v_i$ of the SR-EDF theory and the gauge angle $\varphi$ starting from Eq. (72-74) of Ref. [6]. Altogether, we obtain:

$$\int_{0}^{2\pi} d\varphi \left( \kappa_{ii}^{*0} \kappa_{ii}^{0} - \delta \kappa_{ii}^* \kappa_{ii}^* \right) N_{ii}(0, \varphi) = n_i^N$$

$$- \int_{0}^{2\pi} d\varphi \left( n_i^0 \kappa_{ii}^{0} - \delta n_i [\varphi] \delta n_i [\varphi] \right) N_{ii}(0, \varphi)$$

$$= (n_i^N (1 - n_i^N) + \delta n_i \delta n_i) .$$

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

### Appendix B: Particle number restoration with recurrence relation

A method, alternative to the above 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

$$|\Phi_0\rangle = \prod_{i=0}^{N} (1 + x_i a_i^\dagger a_i^\dagger) |0\rangle ,$$

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

$$|\Psi_N\rangle \propto \left( \sum_{i=0}^{N} x_i a_i^\dagger a_i^\dagger \right)^N |0\rangle .$$

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

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

$$R_{ijj} = N|x_i|^2 \frac{I_{N-1}(i, j)}{I_N} \text{ for } (i \neq j) ,$$

$$R_{ijij} = N(N-1)|x_i|^2 |x_j|^2 \frac{I_{N-3}(i, j)}{I_N} ,$$

while as already mentioned $R_{iijj} = n_i^N$. The different coefficients entering in $n_i^N$ and $R_{ijj}$ are given by:

$$I_K(i) = \sum_{(i_1, \ldots, i_K)} |x_{i_1}|^2 \cdots |x_{i_K}|^2$$

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

$$\cdots$$

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 Variation After Projection (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 (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

$$I_K(i) = I_K - (K - 1)|x_i|^2 I_{K-1}(i)$$

$$I_K = \sum_i |x_i|^2 I_{K-1} - (K - 2) \sum_i |x_i|^4 I_{K-2}(i) .$$

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]:

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

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

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