Configuration mixing within the energy density functional formalism: Removing spurious contributions from nondiagonal energy kernels

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Multi reference calculations along the lines of the generator coordinate method or the restoration of broken symmetries within the nuclear energy density functional (EDF) framework are becoming a standard tool in nuclear structure physics. These calculations rely on the extension of a single-reference energy functional, of the Gogny or the Skyrme types, to nondiagonal energy kernels. There is no rigorous constructive framework for this extension so far. The commonly accepted way proceeds by formal analogy with the expressions obtained when applying the generalized Wick theorem to the nondiagonal matrix element of a Hamilton operator between two product states. It is pointed out that this procedure is ill defined when extended to EDF calculations as the generalized Wick theorem is taken outside of its range of applicability. In particular, such a procedure is responsible for the appearance of spurious divergences and steps in multi reference EDF energies, as was recently observed in calculations restoring particle number or angular momentum. In the present work, we give a formal analysis of the origin of this problem for calculations with and without pairing, i.e., constructing the density matrices from either Slater determinants or quasiparticle vacua. We propose a method to regularize nondiagonal energy kernels such that divergences and steps are removed from multi reference EDF energies. Such a removal is a priori quasiparticle-basis dependent. A special feature of the method we use to proceed to the actual regularization is that it singles out one basis among all possible ones. The regularization method is applicable to calculations based on any symmetry restoration or generator coordinate but is limited to EDFs depending only on *integer* powers of the normal and anomalous density matrices. Eventually, the method is formally illustrated for particle-number restoration and is specified to configuration mixing calculations based on Slater determinants.

I. INTRODUCTION

The nuclear energy density functional (EDF) approach is the microscopic tool of choice to study medium-mass and heavy nuclei in a systematic manner [1]. The EDF approach used in nuclear physics has formal similarities with density functional theory (DFT) [2–8] that provides a formal framework to obtain the exact ground-state energy and one-body density of electronic many-body systems in condensed-matter physics and quantum chemistry [9]. However, and even if it is often referred to as *nuclear DFT* [10–15], the nuclear EDF method has deeply rooted conceptual differences with standard DFT; e.g., Ref. [16].

One of the major challenges of the nuclear many-body problem is that atomic nuclei are self-bound strongly correlated composite systems that tend to display strong collective modes and individual excitations on the same energy scale. This makes the modeling of nuclei differ from that of electronic systems in external potentials to which DFT is heavily applied. The underlying assumption to nuclear EDF approaches is that

correlations can be divided into different classes that can be incorporated through successive refinements of the method. While short-range in-medium correlations are subsumed into a suitable energy density functional, long-range correlations associated with collective modes must be incorporated more explicitly. On this basis, two different levels of EDF calculations coexist in nuclear physics.

On the first level, inappropriately called self-consistent *mean-field* theory, the EDF is constructed from a one-body density matrix that corresponds to a single product state. This reference state is either taken as a Slater determinant, abusively referred to as Hartree-Fock (HF) state, or as a quasiparticle product state, abusively referred to as Hartree-Fock-Bogoliubov (HFB) state. In the present work, this level of description will be referred to as the single reference energy density functional (SR-EDF) method. Within the SR-EDF approach, static correlations associated with collective modes are incorporated through the use of a symmetry-breaking product state.

On the second level, several of those symmetry-breaking product states are mixed in the framework of the generator coordinate method (GCM) with the aim of restoring broken symmetries, allowing for fluctuations of the order parameters of broken symmetries or both. Such a multi reference (MR) EDF approach allows one to incorporate correlations

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TABLE I. List of acronyms repeatedly used in the text.

DFT	density functional theory
EDF	energy density functional
SWT	standard Wick theorem
GWT	generalized Wick theorem
SR	single reference
MR	multi reference
PNR	particle-number restoration
PNP	particle-number projection
BMZ	Bloch-Messiah-Zumino

associated with large amplitude collective motion beyond the static correlations that are easily treated within the SR-EDF method. The energy functional at play in MR-EDF calculations depends on the transition density matrices constructed from all possible pairs of product states that enter the MR set.

Until now, there exists neither a rigorous formal framework underlying MR-EDF calculations nor a guidance from DFT. Indeed, the nuclear MR-EDF method is outside the scope of existing implementations of the Hohenberg-Kohn theorem, even of those dealing specifically with symmetry breaking issues [17–20]. As far as motivating MR-EDF calculations based on the GCM, hybrid approaches used in electronic systems that combine a density functional for diagonal energy kernels and (sometimes scaled) matrix elements of the bare Coulomb force for off-diagonal ones [21] have to be ruled out because of the different nature of the nuclear force and the more complex correlations it induces in the nuclear medium. There is a consensus among practitioners that the SR-EDF should be recovered for any diagonal energy kernel appearing in the MR-EDF and that the nondiagonal kernels should be extrapolated from the SR-EDF on the basis of the generalized Wick theorem (GWT) [22] that provides an efficient tool to evaluate the matrix elements of any operator between two different product states. For diverse reasons, however, SR and MR-EDFs do not reduce to matrix elements of a Hamiltonian operator between many-body states. As a consequence, the procedure outlined above to generate the MR-EDF is not free from problems and inconsistencies.

The present article is the first article of a trilogy where we address one of the problems arising from the current lack of a stringent and consistent constructive framework for the MR-EDF method, namely the appearance of divergences and finite steps that have been recently identified in the context of particle-number restoration (PNR) [23–27]. We propose here a general cure for any type of configuration mixing. In Ref. [28] the method is applied to PNR while in Ref. [29] the specific case of an EDF depending of noninteger powers of the density matrix is discussed. The spurious steps and divergences arise typically as one scans the symmetry-restored energy as a function of a certain degree of freedom; e.g., looking at the PNR potential energy surface of a nucleus as a function of axial quadrupole deformation. For reasons that will become clear below, pure PNR is the only case where the divergent contributions to the energy functional can be traced back

rather easily although no practical solution to this problem has been proposed so far. It is important to realize, however, that similar problems may appear for *any* MR calculation performed within the EDF framework, although they will be hidden in the formal expressions and may be masked by the numerical representation. A pathology that resembles the one identified for PNR has recently been seen in EDF calculations, without explicit treatment of pairing, aiming at restoring angular momentum [30], whereas a similar problem was identified much earlier in the GCM-type mixing of zero- and two-quasiparticle states [31].

It is essential to state that these difficulties are inherent to the EDF formulation of MR calculations and do not exist when the energy relates to the strict average value of a Hamiltonian in a wave function [23–25]. As the major part of the article consists of lengthy formal manipulations that will be easier to follow if anticipating the results, we now summarize the three goals of the present work:

(i) We want to introduce a formal framework that allows the unambiguous identification of terms in the EDF that are responsible for divergences and finite steps in MR-EDF calculations, irrespective of the nature of the configuration mixing involved. As will be shown below, finding the canonical basis of the Bogoliubov transformation that links two HFB states allows us to do so. In that basis, the nondiagonal energy kernel associated with those two vacua and that enters the MR energy can be constructed on the basis of the standard Wick theorem (SWT) instead of the generalized Wick theorem. This will be the key to our analysis.

(ii) Guided by the strict Hamiltonian case, several sources of problems, including those responsible for divergences and steps, are unambiguously identified within the EDF context.

(iii) We provide a minimum but general solution to the problem of divergences and steps in MR-EDF calculations for a particular class of energy functionals. To that end, we propose a correction that removes exactly the difference between the GWT-based and the SWT-based nondiagonal energy kernels. The latter correction preserves the continuity condition between SR- and MR-EDFs. Finally, we provide explicit expressions for particle-number restoration and mixing of Slater determinants.

The article is organized as follows: Section II briefly reviews general aspects of nuclear EDF approaches. Section III is devoted to the actual introduction to SR- and MR-EDF methods. First, the relevant similarities and key differences between Hamiltonian-based calculations and EDF ones are worked out. Second, the connection between the SR functional and the nondiagonal energy kernels at play in the MR formalism is discussed. In Sec. IV, we demonstrate that the usual definition of nondiagonal energy kernels based on the GWT leads to ill-defined calculations when performed within the EDF approach. In Sec. V we propose a correction removing the spurious contributions to the energy functional that is applicable to any MR-EDF calculation. The correction is discussed in detail in Secs. VI and VII for two applications

of current interest. Conclusions and perspectives are given in Sec. VIII.

II. GENERAL ASPECTS OF THE NUCLEAR EDF APPROACH

The nuclear energy density functional integrates out short-range correlations associated with noncollective excitations on a given vacuum, in particular the strong tensor correlations from the vacuum nucleon-nucleon force, thereby introducing higher-order density dependencies into the energy functional. The diagrams that are summed up in the particle-hole and particle-particle channels are different [32,33], which strongly suggests the use of different effective vertices in those two channels of the EDF. Lacking an explicit connection to first principles, existing functionals are constructed using the symmetries of the nuclear Hamiltonian as a guiding principle, whereas their parametrizations are adjusted phenomenologically [1].

Allowing the reference state to break the symmetries of the eigenstates of the underlying Hamiltonian is a way to incorporate *static* long-range correlations associated with collective modes, as, for example, deformation and pairing, with very moderate effort. However, the breaking of symmetries (translational, rotational, parity, and particle number, to name the most current ones) forbids a trivial connection of the nuclear SR-EDF formalism to the Hohenberg-Kohn (HK) theorem that is the foundation of DFT [16]. Indeed, the density that minimizes the exact HK energy functional must reflect the symmetries of the exact ground state of the system. In fact, the appearance of symmetry-breaking solutions in nuclear EDF calculations underlines two important elements: (i) it is crucial and numerically not too difficult to grasp the most important *static* correlations using rather simple approximate functionals and a single-determinantal reference state, at the price of violating the HK theorem, and (ii) kinematical correlations associated with the corresponding symmetry modes (Goldstone modes) as well as the correlations due to the fluctuation of their order parameters are extremely difficult to incorporate into a single-determinantal approach. In other words, correlations associated with highly nonlocal processes such as large-amplitude collective motions can hardly be described within a SR approach based on a standard, nearly local EDF.

It is possible to improve on the SR level by extending the EDF formalism to a multi reference framework, inappropriately referred to as *beyond-mean-field* calculations in the literature. In a MR calculation, a set of (usually) nonorthogonal product states of reference are combined to construct a more general energy functional that involves the computation of nondiagonal norm overlaps and energy kernels between all pairs of vacua. Such MR-EDF calculations are inspired by projection techniques and the GCM whose formalisms are well documented for Hamiltonian-based calculations [34–37]. Symmetry restoration and GCM provide an efficient way to incorporate both collective and single-particle dynamics into a coherent quantum-mechanical formulation. In particular, the GCM allows the inclusion of correlations associated with the

fluctuation of the order parameters of the broken symmetries. Group theoretical considerations [38], the random-phase approximation limit of GCM-type EDF calculations [39], as well as the requirement of continuity between SR and MR functionals discussed in the introduction can be used to constrain the form of the energy kernels to be used in a MR formalism. In particular, it can be shown that the latter energy kernels have to be constructed exclusively from *transition* normal and anomalous one-body density matrices, cf. Eqs. (14)–(16) below, between the two reference states involved. These transition density matrices, however, are at the origin of a major difficulty that arises in existing implementations of MR-EDF calculations.

It is noteworthy that the description of particular systems and phenomena in electronic systems also calls for extensions of the Kohn-Sham implementation of HK-DFT to deal with symmetry-breaking solutions [17–20]. The latter extensions are still connected to the HK theorem and differ from MR-EDF calculations performed in nuclear physics to restore broken symmetries.

III. FROM SINGLE-REFERENCE TO MULTI REFERENCE FUNCTIONAL FRAMEWORKS

We consider the nuclear Hamiltonian under the form

$$H = \sum_{ij} t_{ij} a_i^+ a_j + \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl}\, a_i^+ a_j^+ a_l\, a_k, \tag{1}$$

which, for the sake of transparency of the chain of arguments below, has been limited to the sum of the kinetic energy and a two-body interaction v_{12}, represented through its antisymmetrized matrix elements $\bar{v}_{ijkl}$. For the moment we also do not distinguish between protons and neutrons. The extension to the case of two nucleon species and three-body or even multibody forces of higher order is straightforward (although cumbersome) and will not influence our conclusions.

It is important to stress at this point that, in the present article, H defined above strictly refers to a "vacuum" nuclear Hamiltonian operator; e.g., its two-body part reproduces nucleon-nucleon scattering data up to relevant laboratory energies. Later in this section we refer to *effective* Hamiltonians, either in the context of a truncated single-particle space or because they resum correlations through an explicit dependence on the density of the system. It happens that replacing the vacuum Hamiltonian H by a genuine operator defined within a truncated single-particle space would not modify the following discussion regarding the technical issue addressed in the present article, whereas using a density-dependent "Hamiltonian" is at the origin of some of the problems we are concerned with.

A. Single-reference framework

In the SR approach, the reference state is taken to be an independent-quasiparticle state $|\Phi_0\rangle$, most conveniently

written as a quasiparticle vacuum

$$|\Phi_0\rangle = \mathcal{C}_0 \prod_\nu \alpha_\nu |0\rangle, \tag{2}$$

where $\mathcal{C}_0$ is a complex normalization coefficient. The set of quasiparticle operators $\{\alpha_\nu, \alpha_\nu^+\}$ is obtained from the complete basis of single-particle operators $\{a_i, a_i^+\}$ through a Bogoliubov transformation characterized by the matrices (U^0, V^0)

$$\alpha_\nu^+ = \sum_i \left(U_{i\nu}^0 a_i^+ + V_{i\nu}^0 a_i \right). \tag{3}$$

The index "0" appearing in $|\Phi_0\rangle$ as well as in U^0 and V^0 denotes an ensemble of collective coordinates that fully characterizes the product state $|\Phi_0\rangle$, either regarding broken symmetries or the average value of a constraining operator. This label is of no explicit importance at the SR level but will become mandatory for MR calculations.

1. Strict HFB approach

In the strict HFB approach [40], the reference state $|\Phi_0\rangle$ approximates the actual ground state of the system in such a way that the approximate energy is obtained through

$$E_0 = \frac{\langle \Phi_0 | H | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle}. \tag{4}$$

Using the SWT [41], Eq. (4) can be expressed as

$$E_0 = \sum_{ij} t_{ij} \rho_{ji}^{00} + \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl} \rho_{ki}^{00} \rho_{lj}^{00}$$
$$+ \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl} \kappa_{ij}^{00*} \kappa_{kl}^{00}, \tag{5}$$

where ρ^{00} is the *intrinsic* (SR) normal one-body density matrix and κ^{00} is the intrinsic anomalous density matrix (also called pairing tensor)

$$\rho_{ij}^{00} \equiv \frac{\langle \Phi_0 | a_j^+ a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = (V^{0*} V^{0T})_{ij}, \tag{6}$$

$$\kappa_{ij}^{00} \equiv \frac{\langle \Phi_0 | a_j a_i | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = (V^{0*} U^{0T})_{ij}, \tag{7}$$

$$\kappa_{ij}^{00*} \equiv \frac{\langle \Phi_0 | a_i^+ a_j^+ | \Phi_0 \rangle}{\langle \Phi_0 | \Phi_0 \rangle} = (V^0 U^{0+})_{ij}, \tag{8}$$

associated with the reference state $|\Phi_0\rangle$. The normal density matrix is Hermitian $\rho_{ij}^{00} = \rho_{ji}^{00*}$, whereas the anomalous density matrix is skew symmetric $\kappa_{ij}^{00} = -\kappa_{ji}^{00}$.

The energy E_0 given by Eq. (5) can be seen as the particular energy functional $E[\rho^{00}, \kappa^{00}, \kappa^{00*}]$ that results from taking the expectation value of the Hamiltonian in the product state. This is what is referred to as the *strict* HFB approximation. The minimization of $E[\rho^{00}, \kappa^{00}, \kappa^{00*}]$ with respect to all independent degrees of freedom (ρ_{ii}^{00} as well as $\rho_{ij}^{00}, \rho_{ij}^{00*}, \kappa_{ij}^{00}$, and κ_{ij}^{00*} for $j < i$), under the constraints that the reference state $|\Phi_0\rangle$ remains a quasiparticle vacuum and that the average particle number $\langle \Phi_0 | \hat{N} | \Phi_0 \rangle / \langle \Phi_0 | \Phi_0 \rangle$ has the fixed value N_0, leads to the HFB equation that determines (U^0, V^0) and the densities.

So far, we have not discussed the characteristics of the nuclear Hamiltonian H. Traditional nucleon-nucleon hard-core potentials are not perturbative [42], which makes any attempt to use the strict HFB approximation to the exact nuclear many-body problem useless. The recently proposed soft-core interactions, however, seem to make the nuclear many-body problem perturbative [43]. Still, one must go beyond lowest order to obtain close to converged results and the strict HFB approximation is not quantitatively viable. The situation is further complicated by the necessity to treat three-body and maybe higher-body forces in the nuclear many-body problem [43–47]. As a consequence, one often resorts to an *effective Hamiltonian* that implicitly incorporates correlations brought by the physics outside the model space used in a given calculation. Traditionally, there are two major classes of effective interactions for self-consistent mean-field calculations that represent two different philosophies and strategies to reduce the nuclear many-body problem to a tractable number of relevant degrees of freedom. There are (i) approaches that can be seen as lowest-order approximations to the interacting shell model [48], formulated in terms of effective (often schematic) Hamiltonians in a strict HFB approach using a schematic shell-model space of a very few spherical harmonic-oscillator j shells [34], (ii) approaches that use the full model space of occupied particles together with a density-dependent effective interaction, which are what is nowadays recognized as an approximation to a more general SR-EDF formalism.

2. EDF approach

The EDF approach builds on the last comment. In the context of an EDF formalism, the reference product state $|\Phi_0\rangle$ used to construct the one-body normal and anomalous density matrices [(6)–(8)] is to be seen as an *auxiliary* state that is not meant to be a good approximation of the actual ground-state wave function, in a similar manner as in DFT for electronic systems [4–9,49]. The EDF and the HFB-like equation that results from its minimization contain higher-order correlations than those provided by the strict Hartree, Fock, and Bogoliubov diagrams written in terms of the vacuum interaction. It is important to note that, as opposed to the strict HFB method, the SR-EDF approach does not rely on the Ritz variational principle in the sense that the minimal energy obtained from an approximate energy functional may be below the actual ground-state energy of the system.

Thus, instead of the expectation value of H, the starting point of the method is an energy functional $\mathcal{E}[\rho^{00}, \kappa^{00}, \kappa^{00*}]$ of the normal and anomalous density matrices. Considering the simple case of a bilinear functional to stay formally close to the strict HFB approach with a two-body interaction, a typical EDF can be written as

$$\mathcal{E}[\rho^{00}, \kappa^{00}, \kappa^{00*}] \equiv \mathcal{E}^\rho + \mathcal{E}^{\rho\rho} + \mathcal{E}^{\kappa\kappa}$$
$$= \sum_{ij} t_{ij} \rho_{ji}^{00} + \frac{1}{2} \sum_{ijkl} \bar{v}_{ijkl}^{\rho\rho} \rho_{ki}^{00} \rho_{lj}^{00}$$
$$+ \frac{1}{4} \sum_{ijkl} \bar{v}_{ijkl}^{\kappa\kappa} \kappa_{ij}^{00*} \kappa_{kl}^{00}. \tag{9}$$

In Eq. (9), the matrix elements of the effective vertex $\bar{v}^{\rho\rho}$ might or might not be antisymmetric; e.g., due to the Slater approximation used to treat the exchange contribution from Coulomb or by dropping specific terms of the Skyrme functional [1]. Due to the antisymmetry of κ, however, only the antisymmetrized part of the vertex is probed in the last term of Eq. (9) and one can always take $\bar{v}^{\kappa\kappa}$ to be antisymmetric, which we will do here. In any case, and even though Eqs. (5) and (9) look very similar, $\bar{v}^{\rho\rho}$ and $\bar{v}^{\kappa\kappa}$ should not be seen as interactions in the real sense and are likely to be different. Of course, they are in principle related to the original vacuum interaction but, in the absence of a constructive framework, the link remains implicit. Popular energy density functionals for calculations along these lines [1] are the nonrelativistic Fayans [12], Gogny [50], and Skyrme [51], as well as the relativistic [52] ones.

B. Multi reference extension

Because the nuclear Hamiltonian is invariant under certain symmetry transformations, the independent quasiparticle state $|\Phi_0\rangle$ should be an eigenstate of appropriate linear combinations of the infinitesimal generators. However, the simultaneous preservation of symmetries and the inclusion of long-range correlations associated with large-amplitude collective motions is impossible within the strict HFB formalism and remains untractable within a SR-EDF formalism. As a result, the product state $|\Phi_0\rangle$ is permitted to spontaneously break the symmetries of the true eigenstates to lead to energetically favored solutions; an ambiguity of mean-field and EDF approaches for which Löwdin coined the notion of "symmetry dilemma" in Ref. [53].

To solve that ambiguity, one resorts to a multi reference extension of the method [1]. The starting point consists of a finite set of product states $\{|\Phi_0\rangle; 0 \in \mathrm{MR}\}$, where $\{0 \in \mathrm{MR}\}$ denotes different realizations of the set of collective coordinates that characterize a reference state. If focusing on symmetry restoration, the states belonging to the MR set correspond to one another by the application of a transformation of the symmetry group under consideration. However, the label of the product states in the MR set can also refer to different values of the order parameter of the broken symmetry; the goal of mixing such states being to incorporate correlations associated with fluctuations of that order parameter. In such a case, the operator that links two vacua in the set is not known analytically.

1. Strict projected-GCM approach

In the strict projection-GCM approach, one constructs the projected-GCM state from the product states in the MR set through

$$|\Psi^k\rangle = \sum_{\{0\}\in \mathrm{MR}} f_0^k |\Phi_0\rangle, \tag{10}$$

where the determination of the weight functions f_0^k is discussed below. The index k denotes that not only the ground state but also excited states can be extracted, by projection,

diagonalization, or both. In the *strict* projection-GCM approximation, the many-body energy is approximated by the average value of the nuclear Hamiltonian in the projected-GCM wave function

$$E^k \equiv \frac{\langle\Psi^k|\hat{H}|\Psi^k\rangle}{\langle\Psi^k|\Psi^k\rangle} \tag{11}$$

$$= \frac{\sum_{\{0,1\}\in \mathrm{MR}} f_0^{k*} f_1^k \, E[0,1]\,\langle\Phi_0|\Phi_1\rangle}{\sum_{\{0,1\}\in \mathrm{MR}} f_0^{k*} f_1^k \,\langle\Phi_0|\Phi_1\rangle}, \tag{12}$$

where the set of energy $E[0,1] \equiv \langle\Phi_0|\hat{H}|\Phi_1\rangle/\langle\Phi_0|\Phi_1\rangle$ and norm $\langle\Phi_0|\Phi_1\rangle$ kernels constitute the basic ingredients of the method. Note that Eq. (12) is nothing but the energy in the (Hamiltonian-based) GCM [35,36]. From a formal point of view, symmetry restoration is a special case of the GCM. Indeed, in that case $|\Psi^k\rangle$ can be expressed as a projector acting on one of the symmetry-breaking product state in the MR set. Whereas in the GCM the weight functions f^k are determined variationally from the Hill-Wheeler-Griffin equation [54,55], they are dictated by properties of the relevant symmetry group when performing symmetry restoration.[1]

The energy kernel $E[0,1]$ can be evaluated through the use of the GWT [22]

$$E_{\mathrm{GWT}}[0,1] = \sum_{ij} t_{ij}\rho_{ji}^{01} + \frac{1}{2}\sum_{ijkl} \bar{v}_{ijkl}\rho_{ki}^{01}\,\rho_{lj}^{01}$$

$$+ \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}\kappa_{ij}^{10*}\kappa_{kl}^{01}. \tag{13}$$

It is essential for the present work to note that Eq. (13) is exactly of the same functional form as Eq. (5), except that *intrinsic* density matrices $\{\rho^{00}, \kappa^{00}, \kappa^{00*}\}$ have been replaced by *transition* density matrices defined as

$$\rho_{ij}^{01} \equiv \frac{\langle\Phi_0|a_j^+ a_i|\Phi_1\rangle}{\langle\Phi_0|\Phi_1\rangle}, \tag{14}$$

$$\kappa_{ij}^{01} \equiv \frac{\langle\Phi_0|a_j a_i|\Phi_1\rangle}{\langle\Phi_0|\Phi_1\rangle}, \tag{15}$$

$$\kappa_{ij}^{10*} \equiv \frac{\langle\Phi_0|a_i^+ a_j^+|\Phi_1\rangle}{\langle\Phi_0|\Phi_1\rangle}, \tag{16}$$

where κ_{ij}^{10*} is in general not the complex conjugate of κ_{ij}^{01} anymore. Given Eq. (13), it is clear that any "diagonal" energy kernel, i.e., obtained for $|\Phi_1\rangle = |\Phi_0\rangle$, is equal to the strict HFB energy, Eq. (5), so that the continuity requirement between the SR energy and MR energy kernels stated in the introduction is trivially fulfilled.

As in the strict HFB approximation, a strict projected-GCM calculation performed in terms of the vacuum nuclear Hamiltonian does not lead to quantitatively satisfactory results for all observables of interest. Still, the restoration of the Galilean invariance of spherical HF states [56,57] was studied within such a scheme; i.e., omitting the density-dependent part of the Gogny interaction and keeping exactly all exchange terms

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[1]The weight functions are fully determined only if the symmetry group is Abelian.

in the computation of MR kernels. In fact, MR calculations employing Hamiltonian operators are rather performed within a limited valence space, in the spirit of the interacting shell model, either of projected-GCM type [58–61] or using more elaborate schemes to select the set of reference states like in the MONSTER and VAMPIR approaches [62–64].

2. EDF approach

To perform quantitatively relevant calculations using the full model space of single-particle states, one has to turn to an energy density functional variant of MR calculations. Guided by Eq. (12), the many-body energy is defined in the MR-EDF approach by

$$\mathcal{E}^k \equiv \frac{\sum_{\{0,1\}\in \mathrm{MR}} f_0^{k*} f_1^k \mathcal{E}[0,1] \langle \Phi_0|\Phi_1\rangle}{\sum_{\{0,1\}\in \mathrm{MR}} f_0^{k*} f_1^k \langle \Phi_0|\Phi_1\rangle}, \qquad (17)$$

which now depends only implicitly on the projected-GCM state of Eq. (10). Indeed, the energy $\mathcal{E}^k$ is not the average value of H, or any genuine operator,[2] in $|\Psi^k\rangle$ and it cannot be re-expressed into Eq. (11). Rather, $\mathcal{E}^k$ is to be seen as a more general functional of all product states belonging to the MR set $\{|\Phi_0\rangle; 0\in \mathrm{MR}\}$ as each energy kernel $\mathcal{E}[0,1]$ is a functional of a pair of states $\{|\Phi_0\rangle; |\Phi_1\rangle\}$ in the set.

Although Eq. (17) provides the general ground to calculate the energy of the system within the MR-EDF formalism, there remains the question of how the energy kernel $\mathcal{E}[0,1]$ should be constructed and what its connection to the SR energy functional $\mathcal{E}[\rho^{00}, \kappa^{00}, \kappa^{00*}]$ introduced in the previous section is. Guided by the structure of the expressions in the strict HFB and GCM theories, Eqs. (5) and (13), practitioners of nuclear EDF methods [25,39,65–68] have used the natural extension $\mathcal{E}[0,1] \equiv \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10*}]$ to define the MR energy kernel entering Eq. (17) from the SR energy functional. Using the bilinear SR functional of Eq. (9) for illustration, this leads to a kernel of the form

$$\mathcal{E}_{\mathrm{GWT}}[0,1] \equiv \sum_{ij} t_{ij}\, \rho_{ji}^{01} + \frac{1}{2}\sum_{ijkl} \bar{v}_{ijkl}^{\rho\rho}\, \rho_{ki}^{01}\, \rho_{lj}^{01}$$
$$+ \frac{1}{4}\sum_{ijkl} \bar{v}_{ijkl}^{\kappa\kappa}\, \kappa_{ij}^{01*}\, \kappa_{kl}^{10}, \qquad (18)$$

which is labeled GWT because the definition $\mathcal{E}[0,1] \equiv \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10*}]$ amounts to using the generalized Wick theorem as a motivation to define the MR energy kernel from the SR-EDF.

Calculations along these lines using realistic EDFs have been performed for the restoration of particle numbers [25,68] and angular momentum of axially deformed HFB states [69–72], of angular momentum of cranked HF states [30,73], and of parity of octupole deformed HFB states [74,75]. Some of those calculations also included a GCM-type configuration

mixing along a collective degree of freedom related to spatial deformation.

Other prescriptions than the simple replacement of ρ_{ki}^{00} with ρ_{ki}^{01} have been tried but were found to lead to unrealistic results [39]. The prescription $\mathcal{E}[0,1] \equiv \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10*}]$ ensures that the continuity requirement between the SR and MR levels of description is fulfilled. For symmetry restorations, it can also be shown that the functional should depend only on transition densities [38].

However, the GWT-based prescription to define $\mathcal{E}[0,1]$ causes serious problems as was recently illustrated for PNR in Refs. [25,26] and confirmed from a different point of view in Ref. [28], after earlier warnings [23,24,31] were not recognized. The most spectacular manifestation relates to the appearance of divergences in the PNR energy when two vacua in the MR set are orthogonal, which in pure PNR applications happens for a relative gauge angle of $\pi/2$ when a pair of single-particle states has the occupation probability of $1/2$ [25]. While this poses no problem in the strict PNP-HFB method [23,24], this makes PNR ill defined within the MR-EDF approach. In fact, the energy functional contains not only divergences when encountering orthogonal vacua but also finite spurious contributions even when the two vacua are not orthogonal [28] as will be illustrated later in the present work. It is the goal of the following sections to introduce a method that allows the identification and removal of these spurious terms from any type of MR-EDF calculations.

It is noteworthy that, to the best of our knowledge, the continuity requirement that is always used as a guiding principle to construct nuclear MR energy kernels is never enforced in MR calculations for electronic systems. There, hybrid approaches that use a density functional for diagonal kernels and the (sometimes scaled) bare Coulomb force for nondiagonal kernels are used instead [19,20,76,77], an approach that is facilitated by the fact that the correlation and exchange parts of the energy are a mere correction to the direct Coulomb interaction in most Coulomb systems.

IV. ENERGY KERNELS IN MR APPROACHES

Although the main point of the present work is to stress the differences between strict HFB/projected-GCM approaches and EDF ones, the analysis of the former does offer the key to the understanding of the problems encountered in the latter. As a result, we first concentrate on the strict projected-GCM method and compare the computation of the energy kernel $\langle \Phi_0|H|\Phi_1\rangle/\langle \Phi_0|\Phi_1\rangle$ as obtained from both the GWT and the SWT in a suitable basis.

A. Notation and preliminary discussion

In this section we summarize the elements that will be needed below for the analysis of MR-EDF calculations. The key ingredient will be to find a (quasiparticle) basis that allows the computation of the energy kernel $\langle \Phi_0|H|\Phi_1\rangle/\langle \Phi_0|\Phi_1\rangle$ in terms of the SWT instead of the commonly used GWT. The question if and how this is possible has been addressed already from various perspectives in the past [36,58,78,79].

---

[2]A density-dependent operator, that is, an operator that depends on the solution, is not considered in the present work as a *genuine* operator.

(i) We write the two vacua involved as products of the two corresponding (different) sets of quasiparticle operators, denoted by α_ν and β_ν, respectively,

$$|\Phi_0\rangle = \mathcal{C}_0 \prod_\nu \alpha_\nu |0\rangle,$$
$$|\Phi_1\rangle = \mathcal{C}_1 \prod_\mu \beta_\mu |0\rangle. \tag{19}$$

The moduli of the two complex constants $\mathcal{C}_0$ and $\mathcal{C}_1$ are fixed by the normalization of the states, while their phases can be set to any value.

(ii) We introduce two sets of matrices (U^0, V^0) and (U^1, V^1) that represent the Bogoliubov transformations between an arbitrary, but common, single-particle basis $\{a_i, a_i^+\}$ and the two sets of quasiparticle states

$$\alpha_\nu^+ \equiv \sum_i \left(U_{i\nu}^0 a_i^+ + V_{i\nu}^0 a_i \right), \tag{20}$$
$$\beta_\nu^+ \equiv \sum_i \left(U_{i\nu}^1 a_i^+ + V_{i\nu}^1 a_i \right). \tag{21}$$

(iii) One realizes that the transformation that expresses the quasiparticle operators $\{\beta_\mu, \beta_\mu^+\}$ associated with $|\Phi_1\rangle$ in terms of the quasiparticle operators $\{\alpha_\nu, \alpha_\nu^+\}$ associated with $|\Phi_0\rangle$ is *canonical*, which means it has the form of a general Bogoliubov transformation

$$\beta_\mu^+ = \sum_\nu \left(A_{\nu\mu}\, \alpha_\nu^+ + B_{\nu\mu} \alpha_\nu \right), \tag{22}$$

with the matrices A and B satisfying (see Appendix E of Ref. [36])

$$A \equiv U^{0^+} U^1 + V^{0^+} V^1, \tag{23}$$
$$B \equiv V^{0^T} U^1 + U^{0^T} V^1. \tag{24}$$

To avoid any misunderstanding in what follows, we stress that the Bogoliubov transformation (22) represented by the A and B matrices has nothing to do with pairing correlations. As a consequence, its ingredients have a particular meaning and interpretation that might seem unusual and unexpected (e.g., see Sec. VII). We also stress that no restriction or symmetry is presently imposed on the reference states $\{|\Phi_0\rangle; 0 \in \mathrm{MR}\}$. They might break time-reversal invariance and have an odd number-parity [80,81] (describing odd nuclei), be two-quasiparticle states (describing diabatic excitations), or be higher quasiparticle states. The only restriction is that all reference states belonging to the MR set have the same definite number parity.

(iv) The matrices A and B defined through Eqs. (22)–(24) can be decomposed into a sequence of three simpler transformations thanks to the Bloch-Messiah-Zumino (BMZ) theorem [82,83]

$$A \equiv D\bar{A}C, \quad B \equiv D^*\bar{B}C. \tag{25}$$

where D (C) is a unitary transformation that only mixes quasiparticle creation/annihilation operators $\{\alpha_\nu^+\}/\{\alpha_\nu\}(\{\beta_\mu^+\}/\{\beta_\mu\})$ among each other, whereas $\bar{A}$

and $\bar{B}$ represent a special Bogoliubov transformation. The transformations D and C of the decomposition (25) introduces two intermediate quasiparticle bases $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$ and $\{\tilde{\beta}_\mu, \tilde{\beta}_\mu^+\}$ with different properties from the two original ones $\{\alpha_\nu, \alpha_\nu^+\}$ and $\{\beta_\mu, \beta_\mu^+\}$. As a quasiparticle vacuum is invariant under a unitary transformation among quasi-particle creation/annihilation operators that define it, one could initially choose $|\Phi_0\rangle$ and $|\Phi_1\rangle$ such that $C = D$. In practice, however, this is usually not the case as $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are constructed independently from each other and have to be seen as given inputs to a MR calculation. Finding the transformation that allowed to set $C = D$ would constitute an effort similar to performing the decomposition (25). The advantage of the Bloch-Messiah-Zumino decomposition of the transformation (A, B) becomes clear when looking at the two intermediate sets of quasiparticle operators $\tilde{\alpha}_\nu^+$ and $\tilde{\beta}_\nu^+$

$$\tilde{\alpha}_\nu^+ \equiv \sum_\mu D_{\mu\nu}\alpha_\mu^+, \quad \tilde{\beta}_\nu^+ \equiv \sum_\mu C_{\nu\mu}^*\beta_\mu^+. \tag{26}$$

The two product states $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are still vacua for the two sets of quasiparticle operators $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$ and $\{\tilde{\beta}_\nu, \tilde{\beta}_\nu^+\}$, respectively. In addition, the transformation expressing the latter in terms of the former takes the simple BCS-like form of a special Bogoliubov transformation

$$\tilde{\beta}_\nu^+ = \bar{A}_{\nu\nu}\, \tilde{\alpha}_\nu^+ + \bar{B}_{\bar{\nu}\nu}\, \tilde{\alpha}_{\bar{\nu}}. \tag{27}$$

The matrices $\bar{A}$ and $\bar{B}$ are 2×2 block-diagonal (after a suitable rearrangement of the sequence of indices), with the nonvanishing blocks $\bar{A}(p)$ and $\bar{B}(p)$ being defined as

$$\bar{A}(p) \equiv \begin{pmatrix} \bar{A}_{pp} & 0 \\ 0 & \bar{A}_{\bar{p}\bar{p}} \end{pmatrix}, \quad \bar{B}(p) \equiv \begin{pmatrix} 0 & \bar{B}_{p\bar{p}} \\ \bar{B}_{\bar{p}p} & 0 \end{pmatrix}, \tag{28}$$

where $\bar{A}_{pp} = \bar{A}_{\bar{p}\bar{p}}$ and $\bar{B}_{p\bar{p}} = -\bar{B}_{\bar{p}p}$. The block-diagonal structure of $\bar{A}$ and $\bar{B}$ shows that the quasiparticles $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$ come in conjugated pairs $(\nu, \bar{\nu})$, whose nature will be discussed below. As usual, the block structure can be used to formally separate the corresponding quasiparticle basis into two halves, even though it is not necessary at this point to specify which quantum number is used to distinguish them. For the rest of the article, we introduce the convention that the label p refers to $\nu > 0$ while $\bar{p}$ refers to $\nu < 0$. Thus, when $\nu = p(\bar{p})$, then $\bar{\nu} = \bar{p}(p)$.

(v) Standard BCS techniques allow us to express $|\Phi_1\rangle$ in terms of $|\Phi_0\rangle$ through

$$|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod_{p>0}(\bar{A}_{pp}^* + \bar{B}_{p\bar{p}}^* \tilde{\alpha}_p^+ \tilde{\alpha}_{\bar{p}}^+)|\Phi_0\rangle, \tag{29}$$

where $\tilde{\mathcal{C}}_{01}$ is a complex normalization factor whose properties will be discussed in Sec. IV B.

There are a few further remarks to be made before we continue. When $\bar{A}_{pp}^* \neq 0$ for all p, Eq. (29) is nothing but Eq. (E.39) of Ref. [36]. However, the form above is also valid when $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are orthogonal, i.e., when at least one pair $(p, \bar{p})$ is such

that $\bar{A}^*_{pp} = 0$ (i.e., $\bar{B}^*_{p\bar{p}} = 1$). This situation corresponds to Eq. (E.38) of Ref. [36] with n even and "blocked" quasiparticles coming in pairs $(p, \bar{p})$.[3] One such case occurs when $|\Phi_1\rangle$ is obtained as a two-quasiparticle excitation $(p_0, \bar{p}_0)$ on top of $|\Phi_0\rangle$. This amounts to having $(\bar{A}_{pp} = 1, \bar{B}_{p\bar{p}} = 0)$ for all pairs but the pair $(p_0, \bar{p}_0)$ for which $(\bar{A}_{p_0 p_0} = 0, \bar{B}_{p_0 \bar{p}_0} = 1)$. In fact, there are two different situations to consider depending on the properties of the matrix D. If the latter is the unit matrix, the two-quasiparticle states created are conjugated *in the original basis* $\{\alpha_\mu, \alpha_\mu^+\}$ used to characterize $|\Phi_0\rangle$. However, other two-quasiparticle excitations on top of $|\Phi_0\rangle$ can be generated by considering a nontrivial D transformation.

The above procedure to express $|\Phi_1\rangle$ with respect to $|\Phi_0\rangle$ is close to the method discussed in Ref. [78], although the latter relies on the Thouless representation of quasiparticle vacua [84] that requires taking a more explicit care of orthogonal states. References [58,78,79] are also dedicated to finding a canonical representation appropriate to nondiagonal overlaps. However, they focus on the more difficult task of finding a basis where both vacua are *simultaneously* put into a canonical form. In the present work, we are interested only in putting the Bogoliubov transformation (A, B) describing the transition between the two vacua into a canonical form but not the vacua themselves.

B. Overlaps and one/two-body contractions

The form given by Eq. (29) is very convenient to express the overlap and the matrix element of operators between the states $|\Phi_0\rangle$ and $|\Phi_1\rangle$. First, let us precise the nature of the normalization constant $\tilde{\mathcal{C}}_{01}$. As already said, the two vacua are usually taken to be normalized through an appropriate choice of $|\mathcal{C}_0|$ and $|\mathcal{C}_1|$ in Eq. (19). Calculating

$$\langle\Phi_1|\Phi_1\rangle = |\tilde{\mathcal{C}}_{01}|^2 \langle\Phi_0|\Phi_0\rangle \prod_{p>0}(|\bar{A}_{pp}|^2 + |\bar{B}_{p\bar{p}}|^2) \quad (30)$$

from Eq. (29) and using that $|\bar{A}_{pp}|^2 + |\bar{B}_{p\bar{p}}|^2 = 1$ for all p, the normalization of the two vacua leads to $|\tilde{\mathcal{C}}_{01}|^2 = 1$. However, the latter result does not fix the phase of $\tilde{\mathcal{C}}_{01}$ that remains when calculating the norm overlap between the two vacua

$$\langle\Phi_0|\Phi_1\rangle = \tilde{\mathcal{C}}_{01} \prod_{p>0} \bar{A}^*_{pp} = \tilde{\mathcal{C}}_{01}\sqrt{\det(\bar{A}^*)}. \quad (31)$$

Equation (31) differs from the well-known Onishi-Yoshida formula [85] by that phase factor $\tilde{\mathcal{C}}_{01}$ that depends on the chosen convention, that is, on the explicit form of the states $|\Phi_0\rangle$ and $|\Phi_1\rangle$ taken as an input of the MR calculation. We will show explicitly in Sec. VI how this works for PNR where the phase $\tilde{\mathcal{C}}_{01}$ can be obtained analytically for all pairs of vacua involved in the calculation. Unfortunately, this is not true for more involved MR calculations, as, for example, when superposing particle-number and angular-momentum restorations together with GCM-type configuration mixings.

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[3]The conjugated pairs $\{\tilde{\alpha}^\dagger_\nu, \tilde{\alpha}^+_{\bar{\nu}}\}$ are *not* necessarily related through time-reversal transformation.

In such a case, one must design numerical methods to follow the phase $\tilde{\mathcal{C}}_{01}$ [59,78,86,87].

For reasons that will become clear in a moment, we define for $p \neq q$ the quantities

$$\langle\Phi_0|\Phi_1, p\rangle \equiv \tilde{\mathcal{C}}_{01} \prod_{\substack{p'>0 \\ p'\neq p}} \bar{A}^*_{p'p'}, \quad (32)$$

$$\langle\Phi_0|\Phi_1, p, q\rangle \equiv \tilde{\mathcal{C}}_{01} \prod_{\substack{p'>0 \\ p'\neq p,q}} \bar{A}^*_{p'p'}, \quad (33)$$

using the notations of Ref. [23]. In Eqs. (32) and (33), $\langle\Phi_0|\Phi_1, p\rangle$ and $\langle\Phi_0|\Phi_1, p, q\rangle$ remain unchanged when substituting p and/or q by $\bar{p}$ and/or $\bar{q}$ in such a way that one can refer to $\langle\Phi_0|\Phi_1, \nu\rangle$ and $\langle\Phi_0|\Phi_1, \nu, \mu\rangle$. Note that the latter overlap does not need to be defined for $\nu = \mu$ or $\nu = \bar{\mu}$ as it cannot appear in such cases. Indeed, this would correspond to removing a conjugated pair twice from $|\Phi_1\rangle$, which would lead to

$$|\Phi_1, \nu, \nu\rangle \propto \tilde{\alpha}_\nu \tilde{\alpha}_{\bar{\nu}}|\Phi_1, \nu\rangle = 0. \quad (34)$$

If needed, such particular cases can be trivially taken into account by extending the notation introduced in Eq. (33) through

$$\langle\Phi_0|\Phi_1, \nu, \nu\rangle = \langle\Phi_0|\Phi_1, \nu, \bar{\nu}\rangle \equiv 0. \quad (35)$$

Starting from Eq. (29), it is now straightforward to calculate one-body contractions in the quasiparticle basis $\{\tilde{\alpha}_\mu, \tilde{\alpha}_\mu^+\}$ using the SWT. Using the notations introduced in Eqs. (31) and (32), one finds that

$$\begin{aligned}
\langle\Phi_0|\tilde{\alpha}_\nu^+\tilde{\alpha}_\mu|\Phi_1\rangle &= \langle\Phi_0|\tilde{\alpha}_\nu^+\tilde{\alpha}_\mu^+|\Phi_1\rangle = 0, \\
\langle\Phi_0|\tilde{\alpha}_\nu\tilde{\alpha}_\mu^+|\Phi_1\rangle &= \delta_{\nu\mu}\langle\Phi_0|\Phi_1\rangle, \\
\langle\Phi_0|\tilde{\alpha}_\nu\tilde{\alpha}_\mu|\Phi_1\rangle &= \delta_{\bar{\nu}\mu}\bar{B}^*_{\bar{\nu}\nu}\langle\Phi_0|\Phi_1, \nu\rangle.
\end{aligned} \quad (36)$$

All two-body contractions are obtained in the same manner and can be written in a compact way using the notation introduced in Eqs. (33) and (35), e.g.,

$$\begin{aligned}
\langle\Phi_0|\tilde{\alpha}_\nu\tilde{\alpha}_\mu\tilde{\alpha}_\gamma\tilde{\alpha}_\delta|\Phi_1\rangle &= \delta_{\bar{\nu}\mu}\delta_{\bar{\gamma}\delta}\bar{B}^*_{\bar{\nu}\nu}\bar{B}^*_{\bar{\gamma}\gamma}\langle\Phi_0|\Phi_1, \nu, \gamma\rangle \\
&\quad - \delta_{\bar{\nu}\gamma}\delta_{\bar{\mu}\delta}\bar{B}^*_{\bar{\nu}\nu}\bar{B}^*_{\bar{\mu}\mu}\langle\Phi_0|\Phi_1, \nu, \mu\rangle \\
&\quad + \delta_{\bar{\nu}\delta}\delta_{\bar{\mu}\gamma}\bar{B}^*_{\bar{\nu}\nu}\bar{B}^*_{\bar{\mu}\mu}\langle\Phi_0|\Phi_1, \nu, \mu\rangle. \quad (37)
\end{aligned}$$

C. More convenient bases

To take advantage of the results obtained in the previous section, one has to express the single-particle creation and annihilation operators $\{a_i, a_i^+\}$ in terms of the quasiparticle operators $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$. Introducing the matrices $\tilde{U}^0 = U^0 D$ and $\tilde{V}^0 = V^0 D$, we have

$$a_i^+ = \sum_\nu \left(\tilde{U}^{0*}_{i\nu}\tilde{\alpha}_\nu^+ + \tilde{V}^0_{i\nu}\tilde{\alpha}_\nu\right). \quad (38)$$

Many formulas derived below will simplify by introducing the quasiparticle wave function associated with the quasiparticle operators $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$

$$\begin{pmatrix} \tilde{\alpha}_\nu^+ \\ \tilde{\alpha}_\nu \end{pmatrix}|0\rangle \equiv \begin{pmatrix} |\phi_\nu\rangle \\ |\varphi_{\bar{\nu}}\rangle \end{pmatrix}, \quad (39)$$

where the choice of labeling the lower component $|\varphi_{\bar{\nu}}\rangle$ with the quantum number of the conjugated state in the other half of the basis is dictated by convenience, as will become clearer in the PNR case discussed in Sec. VI.

The upper and lower components can be expressed in terms of the arbitrary single-particle basis $\{a_i, a_i^+\}$ through

$$|\phi_\nu\rangle = \sum_i \tilde{U}_{\nu i}^{0T} |i\rangle, \qquad (40)$$

$$|\varphi_{\bar{\nu}}\rangle = \sum_i \tilde{V}_{\nu i}^{0+} |i\rangle. \qquad (41)$$

We recall that $\tilde{U}^0$ and $\tilde{V}^0$ introduced above involve a unitary transformation D determined by the Bloch-Messiah-Zumino decomposition of the Bogoliubov transformation (A, B). These definitions will allow us to use matrix elements of the effective vertices $\bar{v}^{\rho\rho}$ and $\bar{v}^{\kappa\kappa}$ written in the mixed basis

of upper and lower components of the quasiparticle states $\{|\phi_\nu\rangle, |\varphi_{\bar{\nu}}\rangle\}$, e.g.,

$$\bar{v}_{\varphi_\nu \varphi_\mu \phi_\lambda \phi_\gamma}^{\rho\rho} \equiv \langle \varphi_\nu \varphi_\mu | \bar{v}^{\rho\rho} | \phi_\lambda \phi_\gamma \rangle$$

$$= \sum_{ijkl} \tilde{V}_{i\bar{\nu}}^0 \tilde{V}_{j\bar{\mu}}^0 \tilde{U}_{k\lambda}^0 \tilde{U}_{l\gamma}^0 \bar{v}_{ijkl}^{\rho\rho}, \qquad (42)$$

which are at variance with those expressed in terms of roman indices (i, j, k, l) that relate to the initial arbitrary basis $\{a_i, a_i^+\}$.

D. Energy kernel from the SWT

Thanks to Eqs. (36) and (37), the contribution $\langle \Phi_0 | v_{12} | \Phi_1 \rangle / \langle \Phi_0 | \Phi_1 \rangle$ to the energy kernel $E_{\text{SWT}}[0, 1]$ calculated through the application of the SWT reads as

$$
\begin{aligned}
E_{\text{SWT}}^{\rho\rho}[0, 1] + E_{\text{SWT}}^{\kappa\kappa}[0, 1] &= \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_\mu \varphi_\nu \varphi_\mu} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \phi_{\bar{\nu}} \varphi_\mu \phi_{\bar{\mu}}} \\
&+ \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_\mu \phi_\nu \varphi_\mu} \bar{B}_{\nu\bar{\nu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \varphi_\mu \phi_{\bar{\mu}}} \bar{B}_{\nu\bar{\nu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \\
&+ \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\mu \varphi_\nu \varphi_\mu \phi_\nu} \bar{B}_{\nu\bar{\nu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\mu \phi_{\bar{\mu}} \phi_\nu \phi_{\bar{\nu}}} \bar{B}_{\nu\bar{\nu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \\
&+ \frac{1}{2} \sum_{\substack{\nu\mu \\ \nu \neq \mu, \bar{\mu}}} \bar{v}_{\varphi_\nu \varphi_\mu \phi_\nu \phi_\mu} \bar{B}_{\nu\bar{\nu}}^* \bar{B}_{\mu\bar{\mu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu, \mu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} + \frac{1}{4} \sum_{\substack{\nu\mu \\ \nu \neq \mu, \bar{\mu}}} \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \phi_\mu \phi_{\bar{\mu}}} \bar{B}_{\nu\bar{\nu}}^* \bar{B}_{\mu\bar{\mu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu, \mu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}. \qquad (43)
\end{aligned}
$$

The terms in Eq. (43) are ordered in such a manner that those in the left column can be later identified with terms bilinear in ρ^{01} when using the GWT, whereas the terms in the right column are related to terms proportional to $\kappa^{10*}\kappa^{01}$. It is essential for the following to note that terms with $\nu = \mu$ or $\nu = \bar{\mu}$ do not appear in the last line of Eq. (43), i.e., they are zero.

E. Energy kernel from the GWT

The use of the SWT for the calculation of MR energy kernels relies on the construction of the very particular basis $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$. All practical applications, however, have used the GWT [22] that typically provides, in any arbitrary single-particle basis, energy kernels of the form given by Eq. (13).

The next step is to compare the expressions of the energy kernel obtained from the SWT and the GWT. Using Eqs. (36) and (38), the transition density matrices are given by

$$\rho_{ji}^{01} = \sum_\nu \tilde{V}_{j\nu}^{0*} \tilde{V}_{i\nu}^0 + \sum_\nu \tilde{U}_{j\nu}^0 \tilde{V}_{i\nu}^0 \bar{B}_{\bar{\nu}\nu}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \qquad (44)$$

$$\kappa_{ji}^{10} = \sum_\nu \tilde{V}_{j\nu}^{0*} \tilde{U}_{i\nu}^0 + \sum_\nu \tilde{U}_{j\nu}^0 \tilde{U}_{i\nu}^0 \bar{B}_{\bar{\nu}\nu}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \qquad (45)$$

$$\kappa_{ij}^{01*} = \sum_\nu \tilde{V}_{i\nu}^0 \tilde{U}_{j\nu}^{0*} + \sum_\nu \tilde{V}_{i\nu}^0 \tilde{V}_{j\nu}^0 \bar{B}_{\bar{\nu}\nu}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \qquad (46)$$

where the running index in the sums refers to the basis $\{\tilde{\alpha}_\nu, \tilde{\alpha}_\nu^+\}$. Inserting Eqs. (44)–(46) into Eq. (13), the two-body part of the energy kernel is obtained from the GWT as

$$
\begin{aligned}
E_{\text{GWT}}^{\rho\rho}[0, 1] + E_{\text{GWT}}^{\kappa\kappa}[0, 1] &= \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_\mu \varphi_\nu \varphi_\mu} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \phi_{\bar{\nu}} \varphi_\mu \phi_{\bar{\mu}}} \\
&+ \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_\mu \phi_\nu \varphi_\mu} \bar{B}_{\nu\bar{\nu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \varphi_\mu \phi_{\bar{\mu}}} \bar{B}_{\nu\bar{\nu}}^* \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}
\end{aligned}
$$

$$+ \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\mu \varphi_\nu \varphi_\mu \phi_\nu} \bar{B}^*_{\nu\bar{\nu}} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\mu \phi_{\bar{\mu}} \phi_\nu \phi_{\bar{\nu}}} \bar{B}^*_{\nu\bar{\nu}} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}$$

$$+ \frac{1}{2} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_\mu \phi_\nu \phi_\mu} \bar{B}^*_{\nu\bar{\nu}} \bar{B}^*_{\mu\bar{\mu}} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \frac{\langle \Phi_0 | \Phi_1, \mu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} + \frac{1}{4} \sum_{\nu\mu} \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \phi_\mu \phi_{\bar{\mu}}} \bar{B}^*_{\nu\bar{\nu}} \bar{B}^*_{\mu\bar{\mu}} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \frac{\langle \Phi_0 | \Phi_1, \mu \rangle}{\langle \Phi_0 | \Phi_1 \rangle},$$

$$(47)$$

where each line of Eq. (47) can be put in correspondence with those of Eq. (43). Expression (43) is recovered term by term from Eq. (47) as one can easily check that

$$\frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \frac{\langle \Phi_0 | \Phi_1, \mu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} = \frac{\langle \Phi_0 | \Phi_1, \nu, \mu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \quad (48)$$

for all pairs (μ, ν) such that $\nu \neq \mu$ or $\nu \neq \bar{\mu}$. However, one is left with additional terms in the last line of Eq. (47), i.e., for $\nu = \mu$ and $\nu = \bar{\mu}$, which have no correspondent in the last line of Eq. (43).

In spite of such an apparent difference, the energy kernel $E_{\text{GWT}}[0, 1]$ is strictly equal to $E_{\text{SWT}}[0, 1]$ when calculated from a genuine Hamilton operator, that is, within the strict projected-GCM approximation. To prove it, let us restart from last line of Eq. (47) and isolate the possible source of discrepancies (i.e., terms with $\nu = \mu$ and/or $\nu = \bar{\mu}$). Considering first the terms coming from $\kappa^{10*}\kappa^{01}$, using the antisymmetry of the interaction and the properties of the matrix $\bar{B}$, we find that

$$\frac{1}{4} \sum_\nu \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \phi_\nu \phi_{\bar{\nu}}} \bar{B}^*_{\nu\bar{\nu}} \bar{B}^*_{\nu\bar{\nu}} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}$$

$$+ \frac{1}{4} \sum_\nu \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \phi_{\bar{\nu}} \phi_\nu} \bar{B}^*_{\nu\bar{\nu}} \bar{B}^*_{\bar{\nu}\nu} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}$$

$$= \frac{1}{2} \sum_\nu \bar{v}_{\varphi_\nu \varphi_{\bar{\nu}} \phi_\nu \phi_{\bar{\nu}}} \bar{B}^*_{\nu\bar{\nu}} \bar{B}^*_{\nu\bar{\nu}} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle} \frac{\langle \Phi_0 | \Phi_1, \nu \rangle}{\langle \Phi_0 | \Phi_1 \rangle}, \quad (49)$$

which happens to cancel out exactly the contributions with $\mu = \bar{\nu}$ originating from $\rho^{01}\rho^{01}$. For this cancellation to occur it is crucial that the *same* interaction is employed in both terms, as it is the case if a genuine Hamiltonian is used. Altogether only the term with $\nu = \mu$ from the $\rho^{01} \rho^{01}$ contributions could not be combined with terms from $\kappa^{10*}\kappa^{01}$. However, thanks to the antisymmetry of the two-body interaction, these terms also cancel out.

Therefore, the prerequisites for a complete matching between estimates of the two-body energy kernel from the SWT and the GWT, independently of the appearance of divergences or not, are that

(i) the same interaction kernel is used in both bilinear terms of the EDF to properly recombine specific terms coming from $\rho^{01}\rho^{01}$ and $\kappa^{10*}\kappa^{01}$ and

(ii) the antisymmetry of the interaction kernel is properly accounted for.

The key point is that none of the two previous conditions are fulfilled in general when constructing a MR-EDF through an *ansatz* of the form of Eq. (18): the matrix elements $\bar{v}^{\rho\rho}_{ijkl}$ are not

necessarily antisymmetric, and $\bar{v}^{\rho\rho}_{ijkl}$ and $\bar{v}^{\kappa\kappa}_{ijkl}$ are in general not the same. Consequently, the kernels $\mathcal{E}_{\text{SWT}}[0, 1]$ and $\mathcal{E}_{\text{GWT}}[0, 1]$ defined in the EDF method by analogy with the Hamiltonian formalism are different, with $\mathcal{E}_{\text{GWT}}[0, 1]$ containing terms that do not appear in $\mathcal{E}_{\text{SWT}}[0, 1]$.

V. CORRECTED ENERGY KERNEL

The observations of the previous section are at the heart of the problems encountered in MR-EDF calculations that rely on the GWT to construct the MR energy kernels from the SR-EDF. Let us analyze the situation further and demonstrate that there exist in fact several levels of problems of different physical origin. This will lead us to advocate the explicit removal of specific contributions to $\mathcal{E}_{\text{GWT}}[0, 1]$ to perform meaningful MR-EDF calculations.

It is crucial to note here that, as the correction procedure proposed in the following is based on an analogy with the Hamiltonian formalism, it can be implemented only for functionals containing integer powers of the density matrices. We will come back to that crucial point when discussing the long-term implications of the present work.

A. Bilinear functional

Let us start with the bilinear energy kernel $\mathcal{E}_{\text{GWT}}[0, 1]$ given by Eq. (18). As already discussed, generalizing the functional to the multi reference case using the GWT as a motivation leads to the same structure as the SR-EDF given in Eq. (9), except that intrinsic densities have been replaced with transition ones. Again, the terms $\mathcal{E}^{\rho\rho}_{\text{GWT}}[0, 1]$ and $\mathcal{E}^{\kappa\kappa}_{\text{GWT}}[0, 1]$ might contain different vertices.

We now introduce more compact expressions of the transition density matrices using the identity $\langle \Phi_0 | \Phi_1 \rangle = \bar{A}^*_{\nu\nu} \langle \Phi_0 | \Phi_1, \nu \rangle$

$$\rho^{01} = \rho^{00} + \tilde{U}^0 \bar{Z} \tilde{V}^{0T}$$
$$\kappa^{01} = \kappa^{00} + \tilde{U}^0 \bar{Z} \tilde{U}^{0T} \quad (50)$$
$$\kappa^{10*} = \kappa^{00*} - \tilde{V}^0 \bar{Z} \tilde{V}^{0T},$$

where ρ^{00} and κ^{00} are the intrinsic density matrices associated with $|\Phi_0\rangle$, whereas the matrix $\bar{Z}$ has nonvanishing matrix elements of the form $\bar{Z}_{\bar{\nu}\nu} = (\bar{B}_{\bar{\nu}\nu} \bar{A}^{-1}_{\nu\nu})^*$. Note that $Z = D\bar{Z}D^* = (BA^{-1})^*$ is nothing but the Thouless matrix [22,84] associated with the Bogoliubov transformation connecting $|\Phi_0\rangle$ and $|\Phi_1\rangle$. Equation (50) is an alternative form to the one given in Appendix E of Ref. [36].

Using the mixed basis introduced in Eqs. (40) and (41), as well as Eqs. (47) and (50), the interaction part of the energy kernel

can be written as

$$\mathcal{E}^{\rho\rho}_{\text{GWT}}[0,1] + \mathcal{E}^{\kappa\kappa}_{\text{GWT}}[0,1] = \frac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\varphi_\nu\varphi_\mu} + \frac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\phi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}} \tag{51}$$

$$+ \frac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\varphi_\mu}\,\bar{Z}_{\nu\bar{\nu}} + \frac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\varphi_\mu\phi_{\bar{\mu}}}\,\bar{Z}_{\nu\bar{\nu}} \tag{52}$$

$$+ \frac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\mu\varphi_\nu\varphi_\mu\phi_\nu}\,\bar{Z}_{\nu\bar{\nu}} + \frac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\mu\phi_{\bar{\mu}}\phi_\nu\phi_{\bar{\nu}}}\,\bar{Z}_{\nu\bar{\nu}} \tag{53}$$

$$+ \frac{1}{2}\sum_{\nu\mu}\bar{v}^{\rho\rho}_{\varphi_\nu\varphi_\mu\phi_\nu\phi_\mu}\,\bar{Z}_{\nu\bar{\nu}}\bar{Z}_{\mu\bar{\mu}} + \frac{1}{4}\sum_{\nu\mu}\bar{v}^{\kappa\kappa}_{\varphi_\nu\varphi_{\bar{\nu}}\phi_\mu\phi_{\bar{\mu}}}\,\bar{Z}_{\nu\bar{\nu}}\bar{Z}_{\mu\bar{\mu}}, \tag{54}$$

where the sums run over all states. It is crucial to realize that the eight terms in Eqs. (51)–(54) are arranged in exactly the same manner as the eight terms in Eq. (43).

1. Correcting for divergences and finite steps

By analogy with the strict projected-GCM case discussed in Sec. IV, the contribution to $\mathcal{E}_{\text{GWT}}[0,1]$ from the terms $\nu = \mu$ and $\nu = \bar{\mu}$ in the last line of Eq. (54) should be zero. However, the contribution encoded into the bilinear term $\rho^{01}\rho^{01}$ is not zero for $\mu = \nu$ in line (54) when the effective vertex $\bar{v}^{\rho\rho}$ is not antisymmetric. Also, the vertices $\bar{v}^{\rho\rho}$ and $\bar{v}^{\kappa\kappa}$ have no reason to be the same in an EDF approach; as a result, the contributions from $\rho^{01}\rho^{01}$ for $\mu = \bar{\nu}$ and $\kappa^{10*}\kappa^{01}$ for $(\mu = \nu, \mu = \bar{\nu})$ no longer cancel out in line (54).

This difficulty is caused by the use of the GWT as a motivation to construct MR energy kernel from the SR-EDF. However, it must be made clear that the GWT itself cannot and should not be blamed for this failure, as it is stretched beyond its applicability when used to motivate the form of an energy kernel that does not correspond to the matrix element of an operator. It is problematic though as the terms that do not cancel out in line (54) are at the origins of the divergencies and steps seen in MR-EDF calculations based on the GWT [26] as discussed in detail in Ref. [28].

As a matter of illustration, we now focus on divergences. Divergences will occur in $\mathcal{E}_{\text{GWT}}[0,1]\langle\Phi_0|\Phi_1\rangle$ if the two vacua involved are orthogonal; i.e., when it exists $|\Phi_0\rangle$ and $|\Phi_1\rangle$ in the MR set such that $\langle\Phi_0|\Phi_1\rangle = 0$. As can be seen from Eq. (31), the overlap $\langle\Phi_0|\Phi_1\rangle$ is zero if at least one of the matrix elements $\bar{A}^*_{pp}$ is zero. Because the nonzero contribution to $\mathcal{E}_{\text{GWT}}[0,1]\langle\Phi_0|\Phi_1\rangle$ coming from the term involving the pair $(p, \bar{p})$ in Eq. (54) is proportional to

$$(\bar{Z}_{p\bar{p}})^2\langle\Phi_0|\Phi_1\rangle = \tilde{\mathcal{C}}_{01}(\bar{B}^*_{p\bar{p}})^2\,\frac{1}{\bar{A}^*_{pp}}\prod_{\substack{p'>0\\p'\neq p}}\bar{A}^*_{p'p'}, \tag{55}$$

it will diverge as $\bar{A}^*_{pp}$ goes to zero, except if another factor $\bar{A}^*_{p'p'}$ in the numerator happens to be zero as well. For particular MR calculations and very specific situations, it is indeed possible that several conjugated pairs $(p, \bar{p}), (p', \bar{p'}), \cdots$ are such that

$\bar{A}^*_{pp} = \bar{A}^*_{p'p'} = \cdots = 0$ at the same time. In such a particular case, there will be no divergence of the MR energy due to dangerous terms in Eq. (54).

A regularized energy kernel is obtained by removing the spurious contributions to $\mathcal{E}^{\rho\rho}_{\text{GWT}}$ and $\mathcal{E}^{\kappa\kappa}_{\text{GWT}}$ that constitute the difference between $\mathcal{E}_{\text{GWT}}[0,1]$ and $\mathcal{E}_{\text{SWT}}[0,1]$. This amounts to removing terms involving only one conjugated pair $(p, \bar{p})$ at a time in Eq. (54)

$$\mathcal{E}^{\rho\rho}_{\text{CG}}[0,1] = \frac{1}{2}\sum_{p>0}\big(\bar{v}^{\rho\rho}_{\varphi_p\varphi_p\phi_p\phi_p} + \bar{v}^{\rho\rho}_{\varphi_{\bar{p}}\varphi_{\bar{p}}\phi_{\bar{p}}\phi_{\bar{p}}}$$

$$- \bar{v}^{\rho\rho}_{\varphi_p\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}} - \bar{v}^{\rho\rho}_{\varphi_{\bar{p}}\varphi_p\phi_{\bar{p}}\phi_p}\big)(\bar{Z}_{p\bar{p}})^2, \tag{56}$$

$$\mathcal{E}^{\kappa\kappa}_{\text{CG}}[0,1] = \sum_{p>0}\bar{v}^{\kappa\kappa}_{\varphi_p\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}}(\bar{Z}_{p\bar{p}})^2, \tag{57}$$

where the sum runs over $p = \nu > 0$ only because all the matrix elements involving a given conjugated pair have been explicitly spelled out.

Some important comments should be made:

(i) The sum of Eqs. (56) and (57) is, of course, zero if the MR energy kernel is obtained as the expectation value of the Hamiltonian, whereas it is nonzero for a general functional energy kernel.

(ii) The correction established through Eqs. (56) and (57) is zero when $|\Phi_0\rangle = |\Phi_1\rangle$. Indeed, the Bogoliubov transformation connecting the two states is trivial in this case, with A being the unit matrix and B being zero. As a result, the correction does not modify the diagonal kernels $\mathcal{E}[0,0]$, which preserves the continuity between the SR functional and MR energy kernels $\mathcal{E}[\rho^{00}, \kappa^{00}, \kappa^{00*}] = \mathcal{E}[0,0]$.

(iii) When pairing is not considered explicitly in the theory, the only terms to remove from Eq. (54) are those obtained from $\rho^{01}\rho^{01}$ for $\mu = \nu$. As already discussed, such terms are indeed different from zero if the vertex $\bar{v}^{\rho\rho}$ is not antisymmetric. As a matter of fact, we believe these terms to be responsible for the divergences seen recently in the restoration of angular momentum from cranked HF states [30]; see Sec. VII.

(iv) The correction to $\mathcal{E}_{\text{GWT}}[0, 1]$ is independent of the normalization factor $\tilde{\mathcal{C}}_{01}$ and therefore of the phase conventions chosen to define the two vacua $|\Phi_0\rangle$ and $|\Phi_1\rangle$. This is so because the ratio $\bar{B}_{\bar{p}p}^*/\bar{A}_{pp}^*$ is independent of $\tilde{\mathcal{C}}_{01}$. However, it should be kept in mind that the kernel $\mathcal{E}_{\text{GWT}}[0, 1]$ is to be multiplied eventually by $\langle\Phi_0|\Phi_1\rangle$ where $\tilde{\mathcal{C}}_{01}$ enters explicitly.

(v) Equations (56) and (57) not only remove possible poles leading to divergences but also correct the energy kernel *away* from those potential poles. It is a crucial result of the present work to realize that current calculations are compromised not only through divergences but also through finite spurious contributions.

(vi) As just said, poles associated to zeros of the norm overlaps are only a part of the problem. From that point of view, the study of Ref. [88] about the nodal lines of the overlap between cranked HFB states rotated by different values of the Euler angles is of prime interest. In Ref. [88], it is shown in particular that the structure of nodal lines becomes richer as the states in the MR set are cranked to higher spins.

2. Correcting for self-interaction processes

In the last section, we have isolated the spurious contributions that are specific to $\mathcal{E}_{\text{GWT}}[0, 1]$ when it is not obtained as the matrix element of the Hamiltonian. In particular, it was argued that the construction of MR energy kernels based on the SWT is safe from divergences and steps. However, there exist other, less dangerous, spurious contributions that are common to $\mathcal{E}_{\text{SWT}}[0, 1]$ and $\mathcal{E}_{\text{GWT}}[0, 1]$. This underlines the fact that the SWT is also stretched beyond its applicability when used to construct EDFs that do not correspond to the matrix element of a genuine operator.

The first of those problems relates to the fact that the matrix elements $\bar{v}^{\rho\rho}$ might not be antisymmetrized. This leads to spurious *self-interaction* processes in the functional; i.e., the fact that a nucleon interacts with itself [89]. The spurious terms not already removed by the correction discussed in the previous section, and that should be zero in $\mathcal{E}[0, 1]$, are obtained for $\nu = \mu = p$ or $\nu = \mu = \bar{p}$ in the terms that are independent of $\bar{Z}$ [line (51)] or linear in $\bar{Z}$ [second and third line (52) and (53)]

$$
\begin{aligned}
\mathcal{E}_{\text{SI}}^{\rho\rho}[0, 1] &\equiv \frac{1}{2} \sum_{p>0} \left(\bar{v}_{\varphi_p\varphi_p\varphi_p\varphi_p}^{\rho\rho} + \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{p}}\varphi_{\bar{p}}\varphi_{\bar{p}}}^{\rho\rho} \right) \\
&+ \frac{1}{2} \sum_{p>0} \left(\bar{v}_{\varphi_p\varphi_p\phi_p\varphi_p}^{\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{p}}\phi_{\bar{p}}\varphi_{\bar{p}}}^{\rho\rho} \right) \bar{Z}_{p\bar{p}} \\
&+ \frac{1}{2} \sum_{p>0} \left(\bar{v}_{\varphi_p\varphi_p\varphi_p\phi_p}^{\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{p}}\varphi_{\bar{p}}\phi_{\bar{p}}}^{\rho\rho} \right) \bar{Z}_{p\bar{p}}.
\end{aligned} \tag{58}
$$

It is clear that these terms are unphysical, as they violate Pauli's principle. This gives a strong motivation to remove them from the energy functional, as is sometimes done in DFT for electronic systems [9,89–92], or to construct energy functionals that are self-interaction-free in the first place [93]. When using the standard correction, this will modify the SR energy density functional to what is called an "orbital-dependent functional" in electronic DFT [94,95] and will lead to equations of motion that are more difficult to solve numerically than the usual ones.

From a phenomenological point of view, the merits of self-interaction corrected energy functionals for electronic DFT have not yet been fully clarified, as they improve some observables, but may degrade others when compared to uncorrected functionals [92]. It has also been pointed out that correcting for the one-body self-interaction might not be sufficient, as there also might be also *n*-body self-interactions as well [92,96].

In the nuclear context, the existence of spurious self-interactions in commonly used energy density functionals has been pointed out before [1,97,98] but was never studied in any detail in the published literature.

3. Correcting for self-pairing processes

The second category of problems common to $\mathcal{E}_{\text{SWT}}[0, 1]$ and $\mathcal{E}_{\text{GWT}}[0, 1]$ is less obvious to isolate. In fact, it differs from the two previous sources of problems in the sense that it is subject to interpretation.

It is based on the observation that in the strict HFB or projected/GCM methods, where the same vertex enters $E^{\rho\rho}[0, 1]$ and $E^{\kappa\kappa}[0, 1]$, the terms corresponding to ($\nu = p; \mu = \bar{p}$) and ($\nu = p; \mu = p$) recombine in Eqs. (51)–(53). As explained in Ref. [28], such a recombination of terms can be interpreted as the fact that two nucleons in a pair of conjugated states ($p, \bar{p}$) cannot gain additional binding energy, as compared to the same EDF calculation with no explicit account of pairing, by scattering onto itself. Such a spurious *self-pairing* process should in principle be excluded from the functional, although the actual impact of these terms on observables is not clear yet.

Compared to GWT-related and self-interaction problems, removing the self-pairing energy does not amount to putting specific terms to zero. On the contrary, the reasoning is to allow certain terms to recombine and to provide a finite, nonzero contribution to the energy kernel. It is the remaining finite contribution that is subject to interpretation. Here, we follow the argument from Ref. [28] mentioned above that takes the calculation without explicit treatment of pairing as a reference point. As a result, the advocated correction amounts to replacing specific matrix elements of $\bar{v}^{\kappa\kappa}$ by the corresponding ones of $\bar{v}^{\rho\rho}$. Eventually, the correction for self-pairing amounts to the subtraction of

$$
\begin{aligned}
&\mathcal{E}_{\text{SP}}^{\kappa\kappa}[0, 1] \\
&\equiv \frac{1}{4} \sum_{p>0} \Big[\big(\bar{v}_{\varphi_p\phi_{\bar{p}}\varphi_p\phi_{\bar{p}}}^{\kappa\kappa} + \bar{v}_{\varphi_{\bar{p}}\phi_p\varphi_{\bar{p}}\phi_p}^{\kappa\kappa} - \bar{v}_{\varphi_p\phi_{\bar{p}}\phi_p\varphi_{\bar{p}}}^{\kappa\kappa} - \bar{v}_{\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}\varphi_p}^{\kappa\kappa} \big) \\
&\quad - \big(\bar{v}_{\varphi_p\phi_{\bar{p}}\varphi_p\phi_{\bar{p}}}^{\rho\rho} + \bar{v}_{\varphi_{\bar{p}}\phi_p\varphi_{\bar{p}}\phi_p}^{\rho\rho} - \bar{v}_{\varphi_p\phi_{\bar{p}}\phi_p\varphi_{\bar{p}}}^{\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}\varphi_p}^{\rho\rho} \big) \Big] \\
&\quad + \frac{1}{4} \sum_{p>0} \Big[\big(\bar{v}_{\varphi_p\varphi_{\bar{p}}\varphi_p\phi_{\bar{p}}}^{\kappa\kappa} + \bar{v}_{\varphi_{\bar{p}}\varphi_p\phi_{\bar{p}}\varphi_p}^{\kappa\kappa} - \bar{v}_{\varphi_p\varphi_{\bar{p}}\phi_p\varphi_{\bar{p}}}^{\kappa\kappa} - \bar{v}_{\varphi_{\bar{p}}\varphi_p\varphi_{\bar{p}}\phi_p}^{\kappa\kappa} \big) \\
&\quad - \big(\bar{v}_{\varphi_p\varphi_{\bar{p}}\varphi_p\phi_{\bar{p}}}^{\rho\rho} + \bar{v}_{\varphi_{\bar{p}}\varphi_p\phi_{\bar{p}}\varphi_p}^{\rho\rho} - \bar{v}_{\varphi_p\varphi_{\bar{p}}\phi_p\varphi_{\bar{p}}}^{\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_p\varphi_{\bar{p}}\phi_p}^{\rho\rho} \big) \Big] \bar{Z}_{p\bar{p}} \\
&\quad + \frac{1}{4} \sum_{p>0} \Big[\big(\bar{v}_{\varphi_p\phi_{\bar{p}}\phi_p\phi_{\bar{p}}}^{\kappa\kappa} - \bar{v}_{\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}\phi_p}^{\kappa\kappa} + \bar{v}_{\phi_p\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}}^{\kappa\kappa} - \bar{v}_{\phi_p\varphi_{\bar{p}}\phi_{\bar{p}}\phi_p}^{\kappa\kappa} \big) \\
&\quad - \big(\bar{v}_{\varphi_p\phi_{\bar{p}}\phi_p\phi_{\bar{p}}}^{\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}\phi_p}^{\rho\rho} + \bar{v}_{\phi_p\varphi_{\bar{p}}\phi_p\phi_{\bar{p}}}^{\rho\rho} - \bar{v}_{\phi_p\varphi_{\bar{p}}\phi_{\bar{p}}\phi_p}^{\rho\rho} \big) \Big] \bar{Z}_{p\bar{p}}
\end{aligned}
$$

$$\tag{59}$$

from the energy kernel, Eqs. (51)–(53). The first two lines correspond to the spurious self-pairing energy on the single-reference level, while the last four lines represent the additional self-pairing energy contributing to multi reference calculations.

4. Chosen strategy

The spurious terms causing divergences and steps, Eqs. (56) and (57), are the consequence of a technical problem, i.e., using the GWT beyond its strict domain of validity. This could in principle be avoided by using directly the standard Wick theorem to define the MR energy kernels, Eq. (43). However, it is not clear at present if this would be numerically feasible. Although the direct evaluation of Eq. (43) might be too costly as it requires the explicit computation of the overlaps $\langle\Phi_0|\Phi_1, \nu, \mu\rangle$ for all pairs of states (ν, μ), calculating the correction, (56) and (57), is not and should become a standard procedure in the future. As we demonstrate in Ref. [28] for pure PNR calculations, correcting $\mathcal{E}_{GWT}[0, 1]$ for divergences and finite steps indeed has a visible effect on the binding energy even when not accidentally hitting a divergence. The correction fluctuates on the order of 1 MeV and leads to much smoother deformation energy curves.

From a practitioner's point of view, it is indeed mandatory to correct for divergences and finite steps as they seriously compromise, even inhibit, meaningful MR calculations. Correcting for self-interaction and self-pairing terms would also be desirable, either through explicit construction of self-interaction and self-pairing free energy functionals or through the correction of existing parametrizations of the functionals. Indeed, such spurious contributions to the energy functional violate the Pauli principle and hence are always unphysical.

However, correcting for self-interaction and self-pairing terms, Eqs. (58) and (59), is a complex issue, both conceptually and computationally, i.e., it modifies the SR functional in such a way that the equations of motion are computationally more difficult to solve. However, it is clear that the impact of self-interaction and self-pairing on observables should be scrutinized. Existing studies in the context of HK-DFT for electronic systems [9,89–92,96] demonstrate that it is not an easy task and that it does not necessarily lead to an improvement of the performance of the functionals. As can be seen from Eqs. (58) and (59), self-interaction and self-pairing are a consequence of the violation of the Pauli principle within a pair of conjugated states. Even when removing both from the energy functional, there remain terms in the energy functional that break the particle exchange (anti-)symmetry between states that are not conjugated. Eventually, it should not be forgotten that there is a price to pay for the enormous calculational simplification that EDF methods bring to the many-body problem. Losing antisymmetry on the level of the two-body density matrix is part of it, and how far it should be restored has to be determined as a compromise between the required precision and the necessary computational cost.

5. Fixing the freedom in the regularization procedure

In any regularization procedure, the quantity that results from isolating and throwing away an infinity necessarily depends on explicit or implicit choices that determine its finite value. In the present case, two elements are essential to fix such a freedom.

First, and as explained above, we *choose* not to subtract finite self-interaction and self-pairing contributions that contaminate both SWT- and GWT-based expressions of MR-EDF kernels. The second element relates to the basis used to proceed to the regularization. Although the GWT can be applied in any quasiparticle basis, which makes it so powerful, the application of the SWT necessitates to find a *specific* basis to express $|\Phi_1\rangle$ in terms of $|\Phi_0\rangle$, which we have managed to do as explained in Sec. IV B. Of course, other bases exist that allow the application of the SWT. One such basis [23,79] relies on diagonalizing the matrix $Z^{0\dagger}Z^1$ rather than on applying the BMZ decomposition to the Bogoliubov transformation connecting $|\Phi_0\rangle$ and $|\Phi_1\rangle$.[4] In the resulting basis, the comparison between SWT- and GWT-based formulae for operators matrix elements works just as explained in Sec. IV E in the sense that terms proportional to $\langle\Phi_0|\Phi_1, \nu\rangle\langle\Phi_0|\Phi_1, \nu\rangle/\langle\Phi_0|\Phi_1\rangle^2$ are present in the GWT-based formula but are absent in the SWT-based one. Removing those terms from the GWT-based kernel would again eliminate divergences and steps. However, this would lead to a different regularized energy kernel as the factors and wave functions weighting such terms are not the same as in the basis we prioritize.[5] Consequently, the choice of the basis used to proceed to the regularization impacts the final regularized kernel. Going from one basis to another amounts to reshuffling finite spurious contributions between the different lines of Eqs. (43) or (47).

Knowing that the regularization procedure is necessarily basis dependent, just as standard self-interaction correction methods in DFT are [89], the arguments that led us to prefer the basis we advocate are twofold. First, given $|\Phi_0\rangle$ and $|\Phi_1\rangle$, the application of the BMZ decomposition defines a unique basis, independently on the actual representation of the two states. On the contrary, using the basis that diagonalizes $Z^{0\dagger}Z^1$ would require an extra argument to choose among the infinite number of vacua that can be used to express $|\Phi_0\rangle$ and $|\Phi_1\rangle$. Second, the basis we propose can always be found, whereas it exists (rare) cases for which one cannot diagonalize the matrix $Z^{0\dagger}Z^1$ [79].

Eventually, the motivated choice of the basis we advocate and the decision to postpone to later the more challenging correction for self-interaction and self-pairing processes are the two elements used to fix the freedom that accompanies the present regularization procedure.

B. Correcting higher-order functionals

The cure proposed in the previous section to the problems faced when constructing a MR energy density functional based on the GWT is specific to bilinear functionals. However, realistic functionals contain higher-order dependencies on the

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[4]In fact, there is an infinity of such bases associated with the freedom to choose the third vacua with respect to which $|\Phi_0\rangle$ and $|\Phi_1\rangle$ must be expressed when using the technics of Refs. [23,79].

[5]One noticeable exception is PNR for which all convenient bases are the same.

density matrices associated with many-body correlations and three-body forces. Those higher-order dependencies generate additional spurious contributions to the energy kernel $\mathcal{E}_{\mathrm{GWT}}[0, 1]$ that also have to be corrected for. The generalization of the strategy that we have followed is straightforward, as long as one considers integer powers of the density matrices. Indeed, one can formally relate them to higher-order multibody forces in the Hamiltonian and identify, as we did for two-body forces, which terms are zero when using the SWT and replaced by nonzero terms when using the GWT. However, working out the SWT becomes lengthy and rather tedious for multibody forces.

Thankfully, one does not need to apply the SWT explicitly but rather proceed backward using the connection between the SWT and the GWT discussed in Sec. IV E. This is more convenient because the GWT is easy to apply to any Hamiltonian. For an N-body force, the SWT is recovered from the GWT by expressing n-body transitions densities, with $n \in [0, N]$, through Eqs. (44)–(46) and by using the identity

$$\frac{\langle\Phi_0|\Phi_1, \nu_1\rangle}{\langle\Phi_0|\Phi_1\rangle} \cdots \frac{\langle\Phi_0|\Phi_1, \nu_n\rangle}{\langle\Phi_0|\Phi_1\rangle} = \frac{\langle\Phi_0|\Phi_1, \nu_1, \ldots, \nu_n\rangle}{\langle\Phi_0|\Phi_1\rangle}, \quad (60)$$

which generalizes in passing the notations introduced in Eqs. (32) and (33) in an obvious manner and which is valid as long as all ν_i's belong to different conjugated pairs. When two or more ν_i's belong to the same conjugated pair, the validity of Eq. (60) is lost and the left-hand side factor should be replaced by $\langle\Phi_0|\Phi_1, \nu_1, \ldots, \nu_n\rangle \equiv 0$. Using such shortcuts, one can obtain an explicit "SWT" form for the matrix element of multibody forces in a very economical way.

Let us illustrate the above strategy for a three-body interaction. This will correspond to complementing the SR-EDF $\mathcal{E}[\rho^{00}, \kappa^{00}, \kappa^{00*}]$ and the energy kernel $\mathcal{E}_{\mathrm{GWT}}[0, 1]$ with a trilinear component. The three-body interaction is written as

$$v_{123} = \frac{1}{36} \sum_{ijklmn} \bar{v}_{ijklmn} a_i^+ a_j^+ a_k^+ a_n a_m a_l, \quad (61)$$

where the three-body force matrix elements are fully antisymmetric. Within the strict projected-GCM approximation, the application of the GWT leads to

$$E_{\mathrm{GWT}}^{\rho\rho\rho}[0, 1] + E_{\mathrm{GWT}}^{\rho\kappa\kappa}[0, 1]$$

$$= \frac{1}{6} \sum_{ijklmn} \bar{v}_{ijklmn} \rho_{li}^{01} \rho_{mj}^{01} \rho_{nk}^{01} + \frac{1}{4} \sum_{ijklmn} \bar{v}_{ijklmn} \rho_{li}^{01} \kappa_{jk}^{10*} \kappa_{mn}^{01}. \quad (62)$$

Operating as described above leads to the expression of the overlap (see Appendix A) as it would be obtained from Eq. (29) using the SWT. Such an expression complements the last line of Eq. (43) for the two-body Hamiltonian.

As before, we now define the trilinear energy kernel $\mathcal{E}_{\mathrm{GWT}}^{\rho\rho\rho}[0, 1]$ and $\mathcal{E}_{\mathrm{GWT}}^{\rho\kappa\kappa}[0, 1]$ within the EDF approach in close analogy to the two terms of Eq. (62). The two contributions are expressed in terms of the effective vertices $\bar{v}^{\rho\rho\rho}$ and $\bar{v}^{\rho\kappa\kappa}$, respectively. Just as for the bilinear parts, $\mathcal{E}_{\mathrm{GWT}}^{\rho\rho\rho}[0, 1]$ and $\mathcal{E}_{\mathrm{GWT}}^{\rho\kappa\kappa}[0, 1]$ need now to be corrected for spurious contributions. Proceeding in a similar way as for the bilinear functional, and using the SWT as a reference point, Eq. (A1), the terms to be removed are

$$\begin{aligned}
\mathcal{E}_{\mathrm{CG}}^{\rho\rho\rho}[0, 1] = \frac{1}{6} \sum_{p>0,\nu} \big(& \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\bar{p}}\phi_{\bar{p}}\phi_{\bar{\nu}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_{p}\varphi_{\bar{\nu}}\phi_{\bar{p}}\phi_{p}\phi_{\bar{\nu}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{p}\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}\phi_{\bar{\nu}}}^{\rho\rho\rho} + \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{\bar{\nu}}\phi_{p}\phi_{p}\phi_{\bar{\nu}}}^{\rho\rho\rho} \\
& + \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\varphi_{\bar{p}}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{\bar{p}}\phi_{p}\phi_{\bar{\nu}}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\varphi_{p}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}}^{\rho\rho\rho} + \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{p}\phi_{p}\phi_{\bar{\nu}}\phi_{p}}^{\rho\rho\rho} \\
& + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{\bar{p}}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\bar{p}}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\rho\rho} + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{p}\phi_{p}\phi_{p}\phi_{p}}^{\rho\rho\rho} \big) (\bar{Z}_{p\bar{p}})^2 \\
+ \frac{1}{6} \sum_{p>0,\nu} \big(& \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\bar{p}}\phi_{\bar{p}}\phi_{\bar{\nu}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_{p}\varphi_{\bar{\nu}}\phi_{\bar{p}}\phi_{p}\phi_{\bar{\nu}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{p}\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}\phi_{\bar{\nu}}}^{\rho\rho\rho} + \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{\bar{\nu}}\phi_{p}\phi_{p}\phi_{\bar{\nu}}}^{\rho\rho\rho} \\
& + \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\varphi_{\bar{p}}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{\bar{p}}\phi_{p}\phi_{\bar{\nu}}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\varphi_{p}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}}^{\rho\rho\rho} + \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{p}\phi_{p}\phi_{\bar{\nu}}\phi_{p}}^{\rho\rho\rho} \\
& + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{\bar{p}}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\bar{p}}\phi_{\bar{p}}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{\bar{p}}\varphi_{p}\phi_{\bar{\nu}}\phi_{\bar{p}}\phi_{p}}^{\rho\rho\rho} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\rho\rho} + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{p}\phi_{\bar{\nu}}\phi_{p}\phi_{p}}^{\rho\rho\rho} \big) (\bar{Z}_{p\bar{p}})^2 \, \bar{Z}_{\bar{\nu}\nu},
\end{aligned} \quad (63)$$

and

$$\begin{aligned}
\mathcal{E}_{\mathrm{CG}}^{\rho\kappa\kappa}[0, 1] = \frac{1}{4} \sum_{p>0,\nu} \big(& \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{p}\varphi_{\bar{\nu}}\phi_{\bar{p}}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{p}\varphi_{\bar{\nu}}\phi_{p}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\bar{p}}\phi_{p}}^{\rho\kappa\kappa} + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\kappa\kappa} \\
& + \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\nu}\phi_{\bar{p}}\phi_{\bar{p}}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\nu}\phi_{\bar{p}}\phi_{p}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\phi_{\nu}\phi_{\bar{p}}\phi_{p}\phi_{p}}^{\rho\kappa\kappa} + \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\phi_{\nu}\phi_{p}\phi_{p}\phi_{\bar{p}}}^{\rho\kappa\kappa} \\
& + \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{p}\phi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{p}}\varphi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{p}\phi_{p}\varphi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} + \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{\bar{p}}\phi_{p}\varphi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} \big) (\bar{Z}_{p\bar{p}})^2 \\
+ \frac{1}{4} \sum_{p>0,\nu} \big(& \bar{v}_{\varphi_{\bar{p}}\varphi_{p}\varphi_{p}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{\bar{p}}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{p}\phi_{\bar{p}}\phi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} + \bar{v}_{\varphi_{p}\varphi_{p}\varphi_{\bar{p}}\phi_{p}\phi_{\bar{\nu}}\phi_{\nu}}^{\rho\kappa\kappa} \\
& + \bar{v}_{\varphi_{\bar{p}}\varphi_{\bar{\nu}}\varphi_{\nu}\phi_{\bar{p}}\phi_{\bar{p}}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{\nu}\phi_{\bar{p}}\phi_{p}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{\nu}\phi_{p}\phi_{p}\phi_{p}}^{\rho\kappa\kappa} + \bar{v}_{\varphi_{p}\varphi_{\bar{\nu}}\varphi_{\nu}\phi_{p}\phi_{p}\phi_{\bar{p}}}^{\rho\kappa\kappa} \\
& + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{\bar{p}}\varphi_{p}\phi_{\bar{\nu}}\phi_{\bar{p}}\phi_{p}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{\bar{p}}\varphi_{p}\phi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\kappa\kappa} - \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\kappa\kappa} + \bar{v}_{\varphi_{\bar{\nu}}\varphi_{p}\varphi_{\bar{p}}\phi_{\bar{\nu}}\phi_{p}\phi_{\bar{p}}}^{\rho\kappa\kappa} \big) (\bar{Z}_{p\bar{p}})^2 \, \bar{Z}_{\bar{\nu}\nu}.
\end{aligned} \quad (64)$$

We have not made use of any antisymmetry properties of the vertices in Eqs. (63) and (64), even though the vertex $\bar{v}^{\rho\kappa\kappa}$ can always be chosen to be antisymmetric, at least with respect to the second and third indices on the one hand and to the fifth and sixth indices on the other.

A few observations similar to those made for the correction of the bilinear functional can be made for the trilinear functional. First, $\mathcal{E}_{\mathrm{CG}}^{\rho\rho\rho}[0, 1]$ and $\mathcal{E}_{\mathrm{CG}}^{\rho\kappa\kappa}[0, 1]$ sum up to zero if, and only if, both effective vertices refer to the same fully antisymmetric three-body interaction. Second, both correction terms are zero for $|\Phi_0\rangle = |\Phi_1\rangle$ and do not modify the underlying diagonal kernel $\mathcal{E}[0, 0]$, keeping valid the link between the SR functional and the MR one $\mathcal{E}[\rho, \kappa, \kappa^*] = \mathcal{E}[0, 0]$. Third, the correction to the functional kernel $\mathcal{E}_{\mathrm{GWT}}[0, 1]$ is independent of the normalization coefficient $\tilde{\mathcal{C}}_{01}$.

Note finally that the three-body terms should also be corrected for spurious self-interaction and self-pairing problems. Expressions equivalent to (58) and (59) can be derived without difficulty for three-body vertices (not shown here).

VI. APPLICATION TO PARTICLE-NUMBER RESTORATION

In the present section, we specify the previous findings to PNR calculations. A more extensive discussion of that particular case, including results of realistic calculations, is presented in Ref. [28]. When considering one kind of particles only, the MR set appropriate to PNR is given by the ensemble of quasiparticle vacua $\{|\Phi_\varphi\rangle; \varphi \in [0, 2\pi]\}$ that correspond to states rotated in gauge space by an angle φ. The MR energy functional that amounts to restoring the particle number N is given by

$$\mathcal{E}^N \equiv \int_0^{2\pi} d\varphi \, \frac{e^{-iN\varphi}}{2\pi \, c_N^2} \mathcal{E}[0, \varphi] \, \langle\Phi_0|\Phi_\varphi\rangle, \tag{65}$$

with

$$c_N^2 = \int_0^{2\pi} d\varphi \, \frac{e^{-iN\varphi}}{2\pi} \langle\Phi_0|\Phi_\varphi\rangle, \tag{66}$$

which is real.

In the previous equations, the state $|\Phi_0\rangle$ is the quasiparticle vacuum at gauge angle $\varphi = 0$. Focusing on projection after variation, such a state is obtained from a self-consistent (possibly constrained) SR calculation. Considering the case of an even-even nucleus, the vacuum state, possibly breaking time-reversal invariance, is written in its canonical basis $\{a_i, a_i^+\}$ as

$$|\Phi_0\rangle = \prod_{p>0}(u_p + v_p \, a_p^+ a_{\bar{p}}^+) |0\rangle, \tag{67}$$

where $|0\rangle$ is the particle vacuum and where $\{u_p; v_p\}$ are real numbers. According to our convention, the product in Eq. (67) only runs over the "positive" half of the basis. The state $|\Phi_0\rangle$ is normalized, with the convention that $u_p^2 + v_p^2 = 1$. To underline the link with previous sections, it is worth pointing out that Eq. (67) corresponds to a state $|\Phi_0\rangle = \mathcal{C}_0 \prod_\nu \alpha_\nu |0\rangle$, where the quasiparticle operators $\{\alpha_\nu, \alpha_\nu^+\}$ are defined through

a BCS-type transformation

$$\alpha_\nu^+ = U_{\nu\nu}^0 a_\nu^+ + V_{\bar{\nu}\nu}^0 a_{\bar{\nu}}, \tag{68}$$

with $\nu = p$ or $\bar{p}$ and where we have defined $v_p \equiv V_{p\bar{p}}^{0*} = -V_{\bar{p}p}^{0*}$ and $u_p \equiv U_{pp}^{0*} = U_{\bar{p}\bar{p}}^{0*}$. The normalization of $|\Phi_0\rangle$ corresponds to $|\mathcal{C}_0|^2 \prod_{p>0} v_p^2 = 1$.

The second vacuum required to construct the energy kernel $\mathcal{E}[0, \varphi]$, i.e., where here $|\Phi_1\rangle \equiv |\Phi_\varphi\rangle$. This state is obtained by rotating $|\Phi_0\rangle$ in gauge space by an angle φ, i.e.,

$$|\Phi_\varphi\rangle = e^{i\varphi\hat{N}}|\Phi_0\rangle = \prod_{p>0}(u_p + v_p e^{2i\varphi} a_p^+ a_{\bar{p}}^+)|0\rangle. \tag{69}$$

From a technical point of view, particle-number restoration is simple because all vacua belonging to the MR set share the same canonical basis. As a result, the Bogoliubov transformation linking any pair of vacua in the set is itself canonical, i.e.,

$$\beta_\nu \equiv e^{i\varphi\hat{N}}\alpha_\nu e^{-i\varphi\hat{N}} = \bar{A}_{\nu\nu}^*\alpha_\nu + \bar{B}_{\bar{\nu}\nu}^*\alpha_\nu^+, \tag{70}$$

with

$$\bar{A}_{\bar{p}\bar{p}}^* = \bar{A}_{pp}^* = e^{-i\varphi}(u_p^2 + v_p^2 e^{2i\varphi}), \tag{71}$$

$$\bar{B}_{p\bar{p}}^* = -\bar{B}_{\bar{p}p}^* = u_p v_p(e^{i\varphi} - e^{-i\varphi}). \tag{72}$$

It is also interesting to compute the transition densities through Eq. (50). For example, it leads for the diagonal normal transition density matrix

$$\rho_{pp}^{0\varphi} = V_{p\bar{p}}^{0*}V_{p\bar{p}}^0 + U_{pp}^0 \frac{\bar{B}_{p\bar{p}}^*}{\bar{A}_{\bar{p}\bar{p}}^*}V_{p\bar{p}}^0 = \frac{v_p^2 e^{2i\varphi}}{u_p^2 + v_p^2 e^{2i\varphi}}, \tag{73}$$

whereas the anomalous ones are obtained in the same way as

$$\kappa_{p\bar{p}}^{0\varphi} = \frac{u_p v_p e^{2i\varphi}}{u_p^2 + v_p^2 e^{2i\varphi}}, \tag{74}$$

$$\kappa_{p\bar{p}}^{\varphi0*} = \frac{u_p v_p}{u_p^2 + v_p^2 e^{2i\varphi}}. \tag{75}$$

Before turning to the correction, let us discuss the relative phase between the two vacua. On the one hand, applying Eq. (31) provides

$$\langle\Phi_0|\Phi_\varphi\rangle = \mathcal{C}_{01} \prod_{p>0} e^{-i\varphi}(u_p^2 + v_p^2 e^{2i\varphi}), \tag{76}$$

whereas, on the other hand, the explicit canonical forms given by Eqs. (67)–(69) lead to $\langle\Phi_0|\Phi_\varphi\rangle = \prod_{p>0}(u_p^2 + v_p^2 e^{2i\varphi})$. Thus, the phase convention associated with the canonical forms is equivalent to having chosen $\mathcal{C}_{01} \prod_{p>0} e^{-i\varphi} = 1$.

The fact that the Bogoliubov transformation (A, B) is canonical from the outset is a specificity of PNR. In particular, it corresponds to having the trivial unitary transformations $C = D = 1$ in Eq. (25). For almost all other cases of interest, however, i.e., angular momentum projection and/or GCM-type multi reference calculations, $\bar{A}$ and $\bar{B}$ cannot be obtained analytically. This means that the matrices A and B must be computed using Eq. (23) for each pair of vacua belonging to the MR set. To this end, methods that will be outlined in Sec. VII have to be applied. Their implementation is underway and will be discussed elsewhere.

Finally, the upper and lower components associated with the quasiparticle operators $\{\tilde{\alpha}_p, \tilde{\alpha}_p^+\}$ introduced through Eqs. (40) and (41) take the form

$$
\begin{aligned}
|\varphi_{\bar{p}}\rangle &= -v_p|\bar{p}\rangle, \quad |\varphi_p\rangle = v_p|p\rangle, \\
|\phi_p\rangle &= u_p|p\rangle, \quad |\phi_{\bar{p}}\rangle = u_p|\bar{p}\rangle,
\end{aligned}
\tag{77}
$$

where $|p\rangle$ and $|\bar{p}\rangle$ denote the single-particle states created by a_p^+ and $a_{\bar{p}}^+$, respectively.

A. Bilinear functional

The different types of spurious contributions to the bilinear energy kernel read in the PNR case as

$$
\mathcal{E}_{\mathrm{CG}}^{\rho\rho}[0, \varphi] = \frac{1}{2} \sum_{p>0} \left(\bar{v}_{pppp}^{\rho\rho} + \bar{v}_{\bar{p}\bar{p}\bar{p}\bar{p}}^{\rho\rho} + \bar{v}_{p\bar{p}p\bar{p}}^{\rho\rho} + \bar{v}_{\bar{p}p\bar{p}p}^{\rho\rho} \right)(u_p v_p)^4
$$
$$
\times \frac{(e^{2i\varphi} - 1)^2}{\left(u_p^2 + v_p^2 e^{2i\varphi}\right)^2}, \tag{78}
$$

$$
\mathcal{E}_{\mathrm{CG}}^{\kappa\kappa}[0, \varphi] = -\sum_{p>0} \bar{v}_{p\bar{p}\bar{p}p}^{\kappa\kappa}(u_p v_p)^4 \frac{(e^{2i\varphi} - 1)^2}{\left(u_p^2 + v_p^2 e^{2i\varphi}\right)^2}, \tag{79}
$$

$$
\mathcal{E}_{\mathrm{SI}}^{\rho\rho}[0, \varphi] = \frac{1}{2} \sum_{p>0} \left(\bar{v}_{pppp}^{\rho\rho} + \bar{v}_{\bar{p}\bar{p}\bar{p}\bar{p}}^{\rho\rho} \right)
$$
$$
\times \left[v_p^4 + 2u_p^2 v_p^4 \frac{(e^{2i\varphi} - 1)}{u_p^2 + v_p^2 e^{2i\varphi}} \right], \tag{80}
$$

$$
\mathcal{E}_{\mathrm{SP}}^{\kappa\kappa}[0, \varphi] = \sum_{p>0} \left[\bar{v}_{p\bar{p}p\bar{p}}^{\kappa\kappa} - \frac{1}{2}\left(\bar{v}_{p\bar{p}p\bar{p}}^{\rho\rho} + \bar{v}_{\bar{p}p\bar{p}p}^{\rho\rho} \right) \right]
$$
$$
\times \left[(u_p v_p)^2 + \left(u_p^4 v_p^2 - u_p^2 v_p^4 \right) \frac{(e^{2i\varphi} - 1)}{u_p^2 + v_p^2 e^{2i\varphi}} \right]. \tag{81}
$$

Subtracting $\mathcal{E}_{\mathrm{CG}}^{\rho\rho}[0, \varphi]$ and $\mathcal{E}_{\mathrm{CG}}^{\kappa\kappa}[0, \varphi]$ from the PNR energy kernel does not call for a modification of the underlying SR functional, whereas removing $\mathcal{E}_{\mathrm{SI}}^{\rho\rho}[0, \varphi]$ and $\mathcal{E}_{\mathrm{SP}}^{\kappa\kappa}[0, \varphi]$ would.

B. Trilinear functional

The spurious contribution to be removed from the GWT-based EDF kernel $\mathcal{E}^{\rho\rho\rho}[0, \varphi, \varphi']$ is given by

$$
\mathcal{E}_{\mathrm{CG}}^{\rho\rho\rho}[0, \varphi, \varphi']
$$
$$
= \frac{1}{6} \sum_{p>0, \nu} \left\{ \bar{v}_{\bar{p}\bar{p}\nu\bar{p}\bar{p}\nu}^{\rho\rho\rho} + \bar{v}_{\bar{p}p\nu\bar{p}p\nu}^{\rho\rho\rho} + \bar{v}_{p\bar{p}\nu p\bar{p}\nu}^{\rho\rho\rho} + \bar{v}_{pp\nu pp\nu}^{\rho\rho\rho} \right.
$$
$$
+ \bar{v}_{\bar{p}\nu\bar{p}\bar{p}\nu\bar{p}}^{\rho\rho\rho} + \bar{v}_{p\nu\bar{p}p\nu\bar{p}}^{\rho\rho\rho} + \bar{v}_{\bar{p}\nu p\bar{p}\nu p}^{\rho\rho\rho} + \bar{v}_{p\nu p p\nu p}^{\rho\rho\rho}
$$
$$
+ \bar{v}_{\nu\bar{p}\bar{p}\nu\bar{p}\bar{p}}^{\rho\rho\rho} + \bar{v}_{\nu\bar{p}p\nu\bar{p}p}^{\rho\rho\rho} + \bar{v}_{\nu p\bar{p}\nu p\bar{p}}^{\rho\rho\rho} + \bar{v}_{\nu pp\nu pp}^{\rho\rho\rho} \left. \right\}
$$
$$
\times (u_p v_p)^4 \frac{(1 - e^{2i\varphi})^2}{\left(u_p^2 + v_p^2 e^{2i\varphi}\right)^2} \rho_{\nu\nu}^{0\varphi'}. \tag{82}
$$

In this expression appears a transition density matrix as defined by Eq. (73) and evaluated at a second gauge angle φ'. This second gauge angle refers to the fact that the isospin degree of freedom must be treated explicitly when correcting the trilinear functional, as there will be terms that are bilinear in one isospin and linear in the other. As a result, both projections on neutron and proton numbers must be considered explicitly. The isospin could be omitted for the bilinear functional because, as long as we do not mix neutron and proton in the mean field and only deal with neutron-neutron and proton-proton pairing, the conjugated states p and $\bar{p}$ always refer to the same isospin and are rotated by the same angle φ in gauge space. In $\mathcal{E}^{\rho\rho\rho}$ and $\mathcal{E}^{\rho\kappa\kappa}$, however, the particle ν may have a different isospin from the one of the pair $(p, \bar{p})$ and a second gauge angle φ' must be attached to it.

Finally, the contribution to be removed from the functional energy kernel $\mathcal{E}^{\rho\kappa\kappa}$ reads as

$$
\mathcal{E}_{\mathrm{CG}}^{\rho\kappa\kappa}[0, \varphi, \varphi'] = \frac{1}{4} \sum_{p>0\nu} \left(\bar{v}_{\nu\bar{p}p\nu p\bar{p}}^{\rho\kappa\kappa} - \bar{v}_{\nu\bar{p}p\nu\bar{p}p}^{\rho\kappa\kappa} + \bar{v}_{\nu p\bar{p}\nu p\bar{p}}^{\rho\kappa\kappa} - \bar{v}_{\bar{p}\bar{p}\nu p\nu\bar{p}}^{\rho\kappa\kappa} \right)(u_p v_p)^4 \frac{(1 - e^{2i\varphi})^2}{\left(u_p^2 + v_p^2 e^{2i\varphi}\right)^2} \rho_{\nu\nu}^{0\varphi'}
$$
$$
+ \frac{1}{4} \sum_{p>0\nu} \left(\bar{v}_{\bar{p}\nu\bar{v}\bar{p}p\bar{p}}^{\rho\kappa\kappa} - \bar{v}_{\bar{p}\nu\bar{v}\bar{p}\bar{p}p}^{\rho\kappa\kappa} - \bar{v}_{p\nu\bar{v}p\bar{p}\bar{p}}^{\rho\kappa\kappa} + \bar{v}_{p\nu\bar{v}pp\bar{p}}^{\rho\kappa\kappa} \right)u_p^2(u_p v_p)^3 \frac{(1 - e^{2i\varphi})^2}{\left(u_p^2 + v_p^2 e^{2i\varphi}\right)^2} \kappa_{\nu\bar{v}}^{\varphi'0*}
$$
$$
+ \frac{1}{4} \sum_{p>0\nu} \left(\bar{v}_{\bar{p}\bar{p}p\bar{p}\nu\bar{v}}^{\rho\kappa\kappa} - \bar{v}_{\bar{p}p\bar{p}\bar{p}\nu\bar{v}}^{\rho\kappa\kappa} + \bar{v}_{\bar{p}p pp\nu\bar{v}}^{\rho\kappa\kappa} - \bar{v}_{pp\bar{p}p\nu\bar{v}}^{\rho\kappa\kappa} \right)v_p^2(u_p v_p)^3 \frac{(1 - e^{2i\varphi})^2}{\left(u_p^2 + v_p^2 e^{2i\varphi}\right)^2} \kappa_{\nu\bar{v}}^{0\varphi'}, \tag{83}
$$

where, again, $\varphi' = \varphi$ if and only if ν and p have the same isospin; otherwise $\varphi' \neq \varphi$.

VII. NO-PAIRING CASE

Multi reference EDF calculations are sometimes performed without an explicit account for pairing correlations; i.e.,

the reference states of the MR set take the form of Slater determinants rather than quasiparticle vacua. We concentrate on such a case in the present section. This is of particular interest because recent MR calculations based on triaxial cranked Slater determinants and aiming at restoring angular momentum displayed divergences [30] that we believe to be related to the problems discussed in the present work.

To investigate the zero-pairing realization of the formalism outlined above we consider a MR energy kernel associated with two Slater determinants $|\Phi_0\rangle$ and $|\Phi_1\rangle$ given by

$$|\Phi_0\rangle = \prod_{i=1}^{N} a_i^+ |0\rangle,$$
$$|\Phi_1\rangle = \prod_{i=1}^{N} b_i^+ |0\rangle, \tag{84}$$

where N represents the number of particles, whereas $\{a_i^+\}_{i=1,N}$ and $\{b_i^+\}_{i=1,N}$ are the creation operators associated with occupied, i.e., hole, single-particle states $\{|a_i\rangle\}_{i=1,N}$ and $\{|b_i\rangle\}_{i=1,N}$, respectively. In the general case, we have expressed the two quasiparticle vacua, Eq. (20), in a common, arbitrary single-particle basis. However, numerical applications often make use of two nonequivalent sets of single-particle states to define the two vacua. This is naturally the case when dealing with Slater determinants. Thus, and as a by-product, the following discussion of the zero-pairing case will sketch how to proceed when the quasiparticle vacua are defined with respect to different single-particle bases.

An important result of the present work (Sec. IV) consists in finding a convenient basis through the BMZ decomposition of the Bogoliubov transformation connecting two quasiparticle vacua, Eq. (27). The Slater determinant limit discussed in the present section offers a chance to illustrate more intuitively how this works.

The single-particle subspace spanned by the $\{|b_i\rangle\}_{i=1,N}$ is *a priori* different from the one spanned by the $\{|a_i\rangle\}_{i=1,N}$. However, it is clear that the subspace spanned by the addition of the two bases is at maximum of dimension $2N$. Therefore, one can always complete the set of hole states of $|\Phi_0\rangle$ by an appropriate choice of N particle states, denoted by $\{|a_{\bar{k}}\rangle\}_{k=1,N}$, in such a way that

$$|b_i\rangle = \sum_{j=1}^{N} |a_j\rangle\langle a_j|b_i\rangle + \sum_{k=1}^{N} |a_{\bar{k}}\rangle\langle a_{\bar{k}}|b_i\rangle. \tag{85}$$

Similarly, one can introduce a set of N particle states for $|\Phi_1\rangle$, denoted by $\{|b_{\bar{k}}\rangle\}_{k=1,N}$ such that

$$|a_i\rangle = \sum_{j=1}^{N} |b_j\rangle\langle b_j|a_i\rangle + \sum_{k=1}^{N} |b_{\bar{k}}\rangle\langle b_{\bar{k}}|a_i\rangle. \tag{86}$$

In practice, the most convenient choice is to associate to each state $|b_i\rangle$ an intermediate state $|d_i\rangle$ given by

$$|d_i\rangle \equiv |b_i\rangle - \sum_{j=1}^{N} |a_j\rangle\,\langle a_j|b_i\rangle. \tag{87}$$

Then, the N states $|a_{\bar{k}}\rangle$ are obtained by a Schmidt orthogonalization of the N states $|d_i\rangle$. If the state $|b_i\rangle$ can be completely described by the hole states of $|\Phi_0\rangle$, the associated $|d_i\rangle$ cancels out and the dimensionality of the considered matrix can be reduced.

We associate the creation operators $a_{\bar{k}}^+$ and $b_{\bar{k}}^+$ to the states $|a_{\bar{k}}\rangle$ and $|b_{\bar{k}}\rangle$, respectively. One has in particular $a_{\bar{k}}|\Phi_0\rangle = 0$ and $b_{\bar{k}}|\Phi_1\rangle = 0$, for all $k = 1, \ldots, N$.

Starting from the truncated space as introduced above, a formalism adapted to MR-EDF calculations with Slater determinants could be introduced without referring to quasiparticles at all. Then, expressions of the functional kernels and the corrections to spurious processes could be obtained directly in the language of particles. However, our present goal is to demonstrate how the formalism written previously in terms of quasiparticles can be directly applied to the particular case where pairing is not considered explicitly. The first step is thus to match the particle creation/annihilation operators with quasiparticle creation/annihilation operators for Slater determinants. Although this can be found in textbooks [36], we present it below for the sake of a self-contained description of our method.

A. From particles to quasiparticles

The matching appropriate to the notation used in previous sections is achieved using the standard quasiparticle representation of Slater determinants. We introduce the two sets of quasiparticle annihilation operators α_ν and β_ν and restart from the general form of the transformations between particles and quasiparticles operators:

$$\begin{pmatrix} \alpha \\ \alpha^+ \end{pmatrix} \equiv \begin{pmatrix} U^{0+} & V^{0+} \\ V^{0T} & U^{0T} \end{pmatrix}_{4N} \begin{pmatrix} a \\ a^+ \end{pmatrix}, \tag{88}$$

and

$$\begin{pmatrix} \beta \\ \beta^+ \end{pmatrix} \equiv \begin{pmatrix} U^{1+} & V^{1+} \\ V^{1T} & U^{1T} \end{pmatrix}_{4N} \begin{pmatrix} b \\ b^+ \end{pmatrix}. \tag{89}$$

Here, the index $4N$ is used to stress that only a specific finite number of quasiparticle states is necessary. The annihilation operators verify $\alpha_\nu|\Phi_0\rangle = 0$ and $\beta_\nu|\Phi_1\rangle = 0$ for $\nu = 1, \ldots, 2N$. It is clear that this relation is fulfilled if α_ν (respectively β_ν) is proportional to a linear combination of hole creation operators of $|\Phi_0\rangle$ (respectively $|\Phi_1\rangle$) or to a combination of its particle annihilation operators. This leads to a simple block structure[6] for the matrices $U^{0/1}$ and $V^{0/1}$

$$U^{0/1} \equiv \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}_{2N}, \quad V^{0/1} \equiv \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}_{2N}, \tag{90}$$

which is obtained thanks to a specific ordering of hole and particle states, that is, we have $\{a_\nu^+\}_{\nu=1,2N} \equiv (\{a_i^+\}_{i=1,N}, \{a_{\bar{t}}^+\}_{t=1,N})$.

B. Bogoliubov transformation between two Slater determinants

To express the matrices A and B associated with the transformation between the two sets of quasiparticles $\{\alpha_\nu, \alpha_\nu^\dagger\}$ and $\{\beta_\mu, \beta_\mu^\dagger\}$ introduced above, we first define the transformation

$$\begin{pmatrix} b \\ b^+ \end{pmatrix} = \begin{pmatrix} R & 0 \\ 0 & R^* \end{pmatrix}_{4N} \begin{pmatrix} a \\ a^+ \end{pmatrix}, \tag{91}$$

---

[6]It is worth mentioning that there is a flexibility in choosing the lower-right block and upper-left blocks of $U^{0/1}$ and $V^{0/1}$, respectively. Here we choose the simplest prescription that in our opinion is also the most convenient in applications.

where R is the overlap matrix that can be schematically written as

$$R \equiv \begin{pmatrix} \{\langle b_i | a_j \rangle\} & \{\langle b_i | a_{\bar{j}} \rangle\} \\ \{\langle b_{\bar{i}} | a_j \rangle\} & \{\langle b_{\bar{i}} | a_{\bar{j}} \rangle\} \end{pmatrix}_{2N} \equiv \begin{pmatrix} \mathcal{A}^T & \mathcal{B}^T \\ \mathcal{X}^+ & \mathcal{Y}^+ \end{pmatrix}_{2N}. \quad (92)$$

The matrices A and B can finally be deduced using Eqs. (88), (89), and (91)

$$A = U^{0+} R^+ U^1 + V^{0+} R^T V^1,$$
$$B = V^{0^T} R^+ U^1 + U^{0^T} R^T V^1, \quad (93)$$

which, using the simple form of $U^{0/1}$ and $V^{0/1}$, leads to

$$A = \begin{pmatrix} \mathcal{A} & 0 \\ 0 & \mathcal{Y} \end{pmatrix}_{2N}, \quad B = \begin{pmatrix} 0 & \mathcal{X} \\ \mathcal{B} & 0 \end{pmatrix}_{2N}. \quad (94)$$

C. Bloch-Messiah-Zumino decomposition

The matrices A and B fulfill all usual relations associated with Bogoliubov transformations. Guided by the standard BMZ theorem, we introduce the two matrices S and T defined as

$$S \equiv B^* B^T,$$
$$T \equiv -AB^+ = B^* A^T. \quad (95)$$

These two matrices play a role similar to that of the normal and anomalous density matrices in the SR case. In particular, we have the following relationships

$$S^2 - S = -TT^+,$$
$$ST = TS^*. \quad (96)$$

However, it should be noted that the matrices S and T are *not* related to the transition density matrices in any trivial way. Using the expression of A and B, S can be written as

$$S = \begin{pmatrix} \mathcal{X}^* \mathcal{X}^T & 0 \\ 0 & \mathcal{B}^* \mathcal{B}^T \end{pmatrix}_{2N} \equiv \begin{pmatrix} \mathcal{S}^X & 0 \\ 0 & \mathcal{S}^B \end{pmatrix}_{2N}, \quad (97)$$

while T takes the form

$$T = \begin{pmatrix} 0 & -\mathcal{A}\mathcal{B}^+ \\ +(\mathcal{A}\mathcal{B}^+)^T & 0 \end{pmatrix}_{2N} \equiv \begin{pmatrix} 0 & \mathcal{T} \\ -\mathcal{T}^T & 0 \end{pmatrix}_{2N}, \quad (98)$$

in such a way that T is antisymmetric as expected. In the following, it will be useful to have a more explicit form of the matrices $\mathcal{S}^X$, $\mathcal{S}^B$, and $\mathcal{T}$. Using Eqs. (92) and (85) and (86) we deduce

$$\mathcal{S}^X_{ij} = +\langle a_i | (1 - \rho^{11}) | a_j \rangle^*,$$
$$\mathcal{S}^B_{\bar{i}\bar{j}} = +\langle a_{\bar{i}} | \rho^{11} | a_{\bar{j}} \rangle, \quad (99)$$
$$\mathcal{T}_{i\bar{j}} = -\langle a_i | \rho^{11} | a_{\bar{j}} \rangle^*.$$

One can see from Eq. (99) that all the information relative to the overlaps between the single-particle wave functions of the two bases is encoded into the three matrices $\mathcal{S}^X$, $\mathcal{S}^B$, and $\mathcal{T}$.

The first step to obtain a BMZ decomposition of A and B is to diagonalize the matrix S. The block diagonal form of S, Eq. (97), shows that the unitary transformation allowing to do so is also block diagonal; i.e., diagonalizing S is achieved by diagonalizing $\mathcal{S}^X$ in the subspace of hole states of $|\Phi_0\rangle$ and $\mathcal{S}^B$ in the subspace of particle states of $|\Phi_0\rangle$. As a result of such a transformation, new hole and particle states are obtained for $|\Phi_0\rangle$, denoted by $|\tilde{a}_i\rangle$ and $|\tilde{a}_{\bar{i}}\rangle$, respectively. We define the corresponding creation and annihilation operators by $\tilde{a}_i^+$ and $\tilde{a}_{\bar{i}}$ as well as the eigenvalues of $\mathcal{S}^X$ and $\mathcal{S}^B$ by λ_i^x and $\lambda_{\bar{i}}^b$, respectively. Expressing the two relationships of Eq. (96) in the basis where S is diagonal leads to

$$\lambda_{\bar{j}}^b(\lambda_{\bar{j}}^b - 1) = -\sum_{i=1}^N |\widetilde{\mathcal{T}}_{i\bar{j}}|^2, \quad (100)$$

$$\lambda_i^x(\lambda_i^x - 1) = -\sum_{\bar{j}=1}^N |\widetilde{\mathcal{T}}_{i\bar{j}}|^2, \quad (101)$$

$$\widetilde{\mathcal{T}}_{i\bar{j}}(\lambda_i^x - \lambda_{\bar{j}}^b) = 0, \quad (102)$$

which shows that $\widetilde{\mathcal{T}}_{i\bar{j}}$ may differ from zero only if $\lambda_i^x = \lambda_{\bar{j}}^b$. Let us now consider the different possible eigenvalues of $\mathcal{S}^X$. There exist three different cases

(i) $\lambda_i^x = 0$: this means that the eigenstate $|\tilde{a}_i\rangle$ of $\mathcal{S}^X$ is orthogonal to all particle states of $|\Phi_1\rangle$ and therefore can be written as a linear combination of the occupied states in $|\Phi_1\rangle$. Equation (101) automatically implies that $\widetilde{\mathcal{T}}_{i\bar{j}} = 0$ for all $\bar{j} = 1, \ldots, N$.

(ii) $\lambda_i^x = 1$: this means that the eigenstate $|\tilde{a}_i\rangle$ is fully contained in the subspace of particle states of $|\Phi_1\rangle$. Again, Eq. (101) implies that $\widetilde{\mathcal{T}}_{i\bar{j}} = 0$ for all $\bar{j} = 1, \ldots, N$.

(iii) $1 < \lambda_i^x < 0$: the corresponding eigenstate is neither entirely contained in the space of particle states of $|\Phi_1\rangle$ nor in the space of its hole states. This also means that at least one matrix element $\widetilde{\mathcal{T}}_{i\bar{j}}$ is nonvanishing for $\bar{j} = 1, \ldots, N$. Accordingly, there exists at least one eigenvalue $\lambda_{\bar{j}}^b$ such that $\lambda_{\bar{j}}^b = \lambda_i^x$.

The same classification could be made for the eigenvalues $\lambda_{\bar{i}}^b$ except that $\lambda_{\bar{i}}^b = 0$ or $\lambda_{\bar{i}}^b = 1$ correspond in this case to eigenstates $|\tilde{a}_{\bar{i}}\rangle$ belonging to particle or hole states of $|\Phi_1\rangle$, respectively.

It could be checked that the diagonalization of S is not affected by a unitary transformation that acts separately among the particle or hole states of $|\Phi_1\rangle$. Indeed, ρ^{11} and $(1 - \rho^{11})$ entering Eq. (99) are invariant under such a unitary transformation, respectively. To advance toward the BMZ decomposition the Bogoliubov transformation (93), one now needs to transform the (quasi-)particle states associated with $|\Phi_1\rangle$. This can be achieved by repeating the above procedure for the new matrices $S' \equiv B^T B^*$ and $T' \equiv B^T A$

$$S' = \begin{pmatrix} \mathcal{B}^T \mathcal{B}^* & 0 \\ 0 & \mathcal{X}^T \mathcal{X}^* \end{pmatrix}_{2N} = \begin{pmatrix} \mathcal{S}'^B & 0 \\ 0 & \mathcal{S}'^X \end{pmatrix}_{2N}, \quad (103)$$

and

$$T' = \begin{pmatrix} 0 & \mathcal{B}^T \mathcal{Y} \\ -(\mathcal{B}^T \mathcal{Y})^T & 0 \end{pmatrix}_{2N} = \begin{pmatrix} 0 & \mathcal{T}' \\ -\mathcal{T}'^T & 0 \end{pmatrix}_{2N}, \quad (104)$$

where the matrix elements now read

$$\mathcal{S}'^{B}_{ij} = +\langle b_i|(1 - \rho^{00})|b_j\rangle,$$

$$\mathcal{S}'^{X}_{\bar{i}\bar{j}} = +\langle b_{\bar{i}}|\rho^{00}|b_{\bar{j}}\rangle^*, \qquad (105)$$

$$\mathcal{T}'_{i\bar{j}} = -\langle b_i|\rho^{00}|b_{\bar{j}}\rangle.$$

The unitary transformation that diagonalizes S' constitutes the second step of the procedure. As for S, the transformation is block diagonal, in such a way that hole and particle states transform among themselves. This leads to a new set of single-particle (eigen-)states denoted by $|\tilde{b}_i\rangle$ and $|\tilde{b}_{\bar{i}}\rangle$. The corresponding eigenvalues of S' are given by λ'^{x}_i and $\lambda'^{b}_{\bar{i}}$. Again, we can classify single-particle states in three categories according to the values of λ'^{b}_i for hole states and to the values of $\lambda'^{x}_{\bar{i}}$ for particle states.

From a practical point of view, no numerical diagonalization of S' is actually needed. Starting from the properties of the states $|\tilde{a}_i\rangle$ and $|\tilde{a}_{\bar{j}}\rangle$ obtained through the diagonalization of S

$$\langle \tilde{a}_i|(1 - \rho^{11})|\tilde{a}_j\rangle^* = \lambda^{x}_i\delta_{ij}, \quad \langle \tilde{a}_{\bar{i}}|\rho^{11}|\tilde{a}_{\bar{j}}\rangle = \lambda^{b}_{\bar{j}}\delta_{\bar{i}\bar{j}}, \quad (106)$$

one can deduce the hole and particle states of $|\Phi_1\rangle$ that diagonalize $\mathcal{S}'^{X}$ and $\mathcal{S}'^{B}$. We consider here the case where the eigenvalues λ^{x}_i and $\lambda^{b}_{\bar{i}}$ differ from zero.[7] With each hole state $|\tilde{a}_i\rangle$, respectively particle state $|\tilde{a}^{+}_{\bar{i}}\rangle$, we associate a new particle state $|\tilde{b}_{\bar{i}}\rangle$, respectively hole state $|\tilde{b}_i\rangle$, of $|\Phi_1\rangle$ through

$$|\tilde{b}_{\bar{i}}\rangle \equiv \frac{1}{\sqrt{\lambda^{x}_i}} \sum_{\bar{k}=1}^{N} |b_{\bar{k}}\rangle\,\langle b_{\bar{k}}|\tilde{a}_i\rangle = \frac{1 - \rho^{11}}{\sqrt{\lambda^{x}_i}}|\tilde{a}_i\rangle, \quad (107)$$

$$|\tilde{b}_i\rangle \equiv \frac{1}{\sqrt{\lambda^{b}_{\bar{i}}}} \sum_{k=1}^{N} |b_k\rangle\,\langle b_k|\tilde{a}_{\bar{i}}\rangle = \frac{\rho^{11}}{\sqrt{\lambda^{b}_{\bar{i}}}}|\tilde{a}_{\bar{i}}\rangle. \quad (108)$$

Those states are

(i) orthonormal and have overlaps with the states diagonalizing S given by

$$\langle \tilde{a}_j|\tilde{b}_{\bar{i}}\rangle = +\left(\lambda^{x}_i\right)^{1/2}\delta_{ij},$$

$$\langle \tilde{a}_{\bar{j}}|\tilde{b}_{\bar{i}}\rangle = +\left(\lambda^{x}_i\right)^{-1/2}\tilde{\mathcal{T}}_{i\bar{j}},$$

$$\langle \tilde{a}_{\bar{j}}|\tilde{b}_i\rangle = +\left(\lambda^{b}_{\bar{j}}\right)^{1/2}\delta_{\bar{i}\bar{j}}, \qquad (109)$$

$$\langle \tilde{a}_j|\tilde{b}_i\rangle = -\left(\lambda^{b}_{\bar{j}}\right)^{-1/2}\tilde{\mathcal{T}}_{j\bar{i}},$$

(ii) eigenstates of $\mathcal{S}'^{B}$ and $\mathcal{S}'^{X}$ and fulfill

$$\langle \tilde{b}_i|(1 - \rho^{00})|\tilde{b}_j\rangle = \lambda^{b}_{\bar{i}}\delta_{ij},$$

$$\langle \tilde{b}_{\bar{i}}|\rho^{00}|\tilde{b}_{\bar{j}}\rangle^* = \lambda^{x}_i\delta_{\bar{i}\bar{j}}, \qquad (110)$$

$$\tilde{\mathcal{T}}'_{j\bar{i}} = \widetilde{\mathcal{T}}_{i\bar{j}}.$$

From the above relation, we deduce in particular that $\lambda'^{b}_i = \lambda^{b}_{\bar{i}}$ and $\lambda'^{x}_{\bar{j}} = \lambda^{x}_j$.

Now, a hole state $|\tilde{b}_i\rangle$ with eigenvalues λ'^{b}_i can now be decomposed as

$$|\tilde{b}_i\rangle = |\tilde{a}_{\bar{i}}\rangle\langle \tilde{a}_{\bar{i}}|\tilde{b}_i\rangle + \sum_{j/\lambda^{x}_j = \lambda'^{b}_i} |\tilde{a}_j\rangle\langle \tilde{a}_j|\tilde{b}_i\rangle, \quad (111)$$

where only the particle state $|\tilde{a}_{\bar{i}}\rangle$ from which $|\tilde{b}_i\rangle$ is constructed appears, while the summation over holes of $|\Phi_0\rangle$ is restricted to states that have the same eigenvalue as $|\tilde{b}_i\rangle$. As a result, the number of states in the expansion is greatly reduced as compared to Eq. (85).

The matrix A is not yet written in a canonical form. To complete the BMZ decomposition, we perform a third transformation consisting of mixing the states $|\tilde{a}_i\rangle$ (respectively $|\tilde{a}_{\bar{i}}\rangle$) within each degenerate subspace of $\mathcal{S}^{X}$ (respectively $\mathcal{S}^{B}$) in such a way that the matrix $\mathcal{A}$ (respectively $\mathcal{Y}$) becomes diagonal. The product of the transformations diagonalizing S and A provides the unitary transformation D introduced in Sec. IV where we explained our method in the general case. As A is being diagonalized, the states $|\tilde{b}_{\bar{i}}\rangle$ (respectively $|\tilde{b}_i\rangle$) are modified accordingly through Eq. (107) [respectively Eq. (108)].[8] Together with the transformation that diagonalized S', this provides the unitary transformation C introduced in Sec. IV.

Finally, the BMZ decomposition of the Bogoliubov transformation between two Slater determinants (93) is achieved in the sense that the matrices

$$\bar{A} \equiv \begin{pmatrix} \bar{\mathcal{A}} & 0 \\ 0 & \bar{\mathcal{Y}} \end{pmatrix}_{2N}, \qquad \bar{B} \equiv \begin{pmatrix} 0 & \bar{\mathcal{X}} \\ \bar{\mathcal{B}} & 0 \end{pmatrix}_{2N}, \qquad (112)$$

are in canonical forms when expressed in the new bases. In the present case, conjugated pairs are made of a particle state $\tilde{a}^{+}_{\bar{i}}$ and a hole state $\tilde{a}^{+}_i$ of $|\Phi_0\rangle$. Through a BCS-like transformation, the latter pair is associated with a unique particle-hole pair $(\tilde{b}^{+}_i, \tilde{b}^{+}_{\bar{i}})$ of $|\Phi_1\rangle$[9]

$$\tilde{b}_i = \bar{\mathcal{A}}_{ii}\,\tilde{a}_i + \bar{\mathcal{B}}_{\bar{i}i}\,\tilde{a}_{\bar{i}}, \qquad (113)$$

$$\tilde{b}^{+}_{\bar{i}} = \bar{\mathcal{X}}_{i\bar{i}}\,\tilde{a}_i + \bar{\mathcal{Y}}_{\bar{i}\bar{i}}\,a^{+}_{\bar{i}}, \qquad (114)$$

where the matrix elements of $\bar{A}$ and $\bar{B}$ are given by the canonical expression

$$\bar{\mathcal{A}}_{ji} \equiv \delta_{ji}\langle \tilde{b}_i|\tilde{a}_i\rangle, \qquad \bar{\mathcal{B}}_{\bar{j}i} \equiv \delta_{\bar{j}i}\langle \tilde{b}_i|\tilde{a}_{\bar{i}}\rangle,$$

$$\bar{\mathcal{X}}_{j\bar{i}} \equiv \delta_{\bar{j}i}\langle \tilde{a}_i|\tilde{b}_{\bar{i}}\rangle, \qquad \bar{\mathcal{Y}}_{\bar{j}\bar{i}} \equiv \delta_{\bar{j}\bar{i}}\langle \tilde{a}_{\bar{i}}|\tilde{b}_{\bar{i}}\rangle. \qquad (115)$$

Finally, Fig. 1 illustrates the procedure and the meaning of putting the Bogoliubov transformation of dimension $2N$ that connects two Slater determinants into a canonical form.

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[7]If the eigenvalue $\lambda^{x}_i/\lambda^{b}_{\bar{i}}$ is 0 or 1, the state $|\tilde{a}_i\rangle/|\tilde{a}_{\bar{i}}\rangle$ is already a particle or a hole state of $|\Phi_1\rangle$. These cases can be treated through a preliminary step where some of the states $|\tilde{b}_i\rangle$ and $|\tilde{b}_{\bar{i}}\rangle$ are directly identified as particle and hole states of $|\Phi_0\rangle$. The other particle and hole states of $|\Phi_1\rangle$ are changed accordingly to fulfill orthogonality conditions.

[8]Although the last step bringing A into a canonical form involves an additional transformation, we use the same notation $\{|\tilde{a}_i\rangle; |\tilde{a}_{\bar{i}}\rangle\}_{i=1,...,N}$ and $\{|\tilde{b}_i\rangle; |\tilde{b}_{\bar{i}}\rangle\}_{i=1,...,N}$ to denote the bases before and after that last transformation.

[9]The bases $\{\tilde{a}_i, \tilde{a}^{\dagger}_i\}$ and $\{\tilde{b}_i, \tilde{b}^{\dagger}_i\}$ are the analog of the bases $\{\tilde{\alpha}_\nu, \tilde{\alpha}^{\dagger}_\nu\}$ and $\{\tilde{\beta}_\mu, \tilde{\beta}^{\dagger}_\mu\}$ defined by Eq. (27) in the general case.
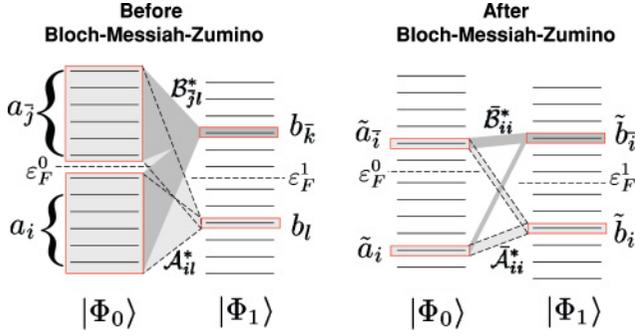
FIG. 1. (Color online) Schematic illustration of the different bases introduced in the text. (Left) The Slater determinants $|\Phi_0\rangle$ and $|\Phi_1\rangle$ are expressed in their respective natural bases $\{|a_i\rangle\}$ and $\{|b_l\rangle\}$. The shaded areas indicate that one state of the basis $\{|b_l\rangle\}$ ($\{|a_i\rangle\}$) is *a priori* spread over all particle and hole states of the basis $\{|a_i\rangle\}$ ($\{|b_l\rangle\}$). (Right) The BMZ decomposition leads to two bases that are such that each transformed state $|\tilde{b}_i\rangle$ ($|\tilde{a}_i\rangle$) decomposes only onto two states $(\tilde{a}_i, \tilde{a}_{\bar{i}})$ $[(\tilde{b}_i, \tilde{b}_{\bar{i}})]$ (one hole and one particle). At the same time, the latter decomposition highlights that the notion of *conjugated* pairs for Slater determinants relates to the association of each hole state with a particular particle state. Note that energy levels have no specific meaning in this figure; they are just meant to characterize occupied and empty levels for each of the Slater determinants.

D. Correction for spurious processes

Given the BMZ decomposition of the transformation between two Slater determinants obtained above, we can apply directly the results derived in Sec. IV, using the new basis $\{\tilde{a}_i, \tilde{a}_i^\dagger\}$, to write the state $|\Phi_1\rangle$ under the form

$$|\Phi_1\rangle = \prod_{i=1}^{N} (\bar{\mathcal{A}}_{ii}^* + \bar{\mathcal{B}}_{i\bar{i}}^* \, \tilde{a}_i \tilde{a}_{\bar{i}}^+)|\Phi_0\rangle, \qquad (116)$$

and the transition density matrix between the two Slater determinants as

$$\rho^{01} = \rho^{00} + \sum_{i=1}^{N} |\tilde{a}_{\bar{i}}\rangle \, \bar{\mathcal{Z}}_{\bar{i}i} \langle \tilde{a}_i|, \qquad (117)$$

where, as before, $\bar{\mathcal{Z}}_{\bar{i}i} \equiv \bar{\mathcal{B}}_{i\bar{i}}^* \, \bar{\mathcal{A}}_{ii}^{*-1}$. As can be seen from Eq. (116), the picture emerging in the new basis is very intuitive because the Slater determinant $|\Phi_1\rangle$ is obtained as a linear combination of up to, very specific, N particle-N hole configurations on the vacuum $|\Phi_0\rangle$. In particular, each hole $\tilde{a}_i$ is combined with a specific particle $\tilde{a}_{\bar{i}}$; the latter association defining the notion of *conjugated pair* for the Bogoliubov transformation that links two Slater determinants. Such an expression simplifies tremendously the general expression connecting two nonorthogonal Slater determinants where each hole state can be excited into any particle states, up to infinite energy.

As for calculations with an explicit treatment of pairing, Eq. (117) can be used to express the MR energy kernel on the basis of the GWT. This leads to

$$\mathcal{E}_{\text{GWT}}[0, 1] = \sum_{i=1}^{N} \left(t_{\tilde{a}_i \tilde{a}_i} + t_{\tilde{a}_i \tilde{a}_{\bar{i}}} \bar{\mathcal{Z}}_{\bar{i}i} \right) + \frac{1}{2} \sum_{i,j=1}^{N} \bar{v}_{\tilde{a}_i \tilde{a}_j \tilde{a}_i \tilde{a}_j}^{\rho\rho}$$

$$+ \frac{1}{2} \sum_{i,j=1}^{N} \left(\bar{v}_{\tilde{a}_i \tilde{a}_j \tilde{a}_{\bar{i}} \tilde{a}_j}^{\rho\rho} + \bar{v}_{\tilde{a}_j \tilde{a}_i \tilde{a}_j \tilde{a}_{\bar{i}}}^{\rho\rho} \right) \bar{\mathcal{Z}}_{\bar{i}i}$$

$$+ \frac{1}{2} \sum_{i,j=1}^{N} \bar{v}_{\tilde{a}_i \tilde{a}_j \tilde{a}_{\bar{i}} \tilde{a}_{\bar{j}}}^{\rho\rho} \bar{\mathcal{Z}}_{\bar{i}i} \, \bar{\mathcal{Z}}_{\bar{j}j}. \qquad (118)$$

Starting from this expression, the self-interaction $\mathcal{E}_{\text{SI}}^{\rho\rho}[0, 1]$ and the spurious contribution to the MR energy due to the construction of the energy kernels on the basis of the GWT $\mathcal{E}_{\text{CG}}^{\rho\rho}[0, 1]$ can be identified

$$\mathcal{E}_{\text{SI}}^{\rho\rho}[0, 1] = \frac{1}{2} \sum_{i=1}^{N} \bar{v}_{\tilde{a}_i \tilde{a}_i \tilde{a}_i \tilde{a}_i}^{\rho\rho}$$

$$+ \frac{1}{2} \sum_{i=1}^{N} \left(\bar{v}_{\tilde{a}_i \tilde{a}_i \tilde{a}_{\bar{i}} \tilde{a}_i}^{\rho\rho} + \bar{v}_{\tilde{a}_i \tilde{a}_i \tilde{a}_i \tilde{a}_{\bar{i}}}^{\rho\rho} \right) \bar{\mathcal{Z}}_{\bar{i}i}, \quad (119)$$

$$\mathcal{E}_{\text{CG}}^{\rho\rho}[0, 1] = \frac{1}{2} \sum_{i=1}^{N} \bar{v}_{\tilde{a}_i \tilde{a}_i \tilde{a}_{\bar{i}} \tilde{a}_{\bar{i}}}^{\rho\rho} \, \bar{\mathcal{Z}}_{\bar{i}i}^2, \qquad (120)$$

whereas, of course, no spurious self-pairing occurs in the present application.

Again, both terms are zero for energy kernels obtained as the matrix element of a Hamiltonian. The latter of the two terms is very likely to be responsible for the difficulties recently encountered in calculations aiming at restoring angular momentum using a MR set of cranked Slater determinants [30]. We thus advocate the removal of the contribution given by Eq. (120) in such a context.

VIII. CONCLUSIONS

The present work concentrates on MR calculations, customarily called "beyond-mean-field" calculations in the literature, performed within the EDF formalism. The multi reference method is nowadays routinely applied with the aim of including long-range correlations associated with large-amplitude collective motions that are difficult to incorporate in a more traditional single-reference (SR), i.e., "mean-field," EDF formalism [1]. So far, the framework for such MR-EDF calculations was set-up by analogy with projection techniques and the GCM that has been rigorously formulated so far only within a Hamiltonian/wave-function-based framework [35,36].

The first achievement of the present work is to demonstrate that the usual extension of the single-reference energy functional $\mathcal{E}[\rho, \kappa, \kappa^*]$ into the nondiagonal energy kernel $\mathcal{E}[0, 1]$ at play in MR calculations through $\mathcal{E}[0, 1] \equiv \mathcal{E}[\rho^{01}, \kappa^{01}, \kappa^{10*}]$ is ill defined. The latter extension, based on the GWT [22] is well defined within a Hamiltonian/wave-function-based projected-GCM framework but happens to be at the origin of spurious divergences and steps in MR-EDF calculations, as

recently realized for particle-number and angular-momentum restorations [25,26,30].

The second achievement of the present article is to propose a method to identify, for any type of symmetry restoration and/or GCM-based calculations, the spurious terms in the MR-EDF responsible for divergences, steps, self-interaction, and self-pairing. The versatility of the method also allows to take care of difficulties encountered when mixing within the MR-EDF calculation states obtained from quasiparticle excitations [31].

In practice, the method requires first putting the Bogoliubov transformation connecting two vacua $|\Phi_0\rangle$ and $|\Phi_1\rangle$ into a canonical form. In the corresponding canonical basis, spurious contributions to the MR energy kernel $\mathcal{E}_{\mathrm{GWT}}[0, 1]$ can be identified and, if necessary, removed. Subtracting the terms responsible for divergences and steps is a prerequisite to perform well-defined multi reference EDF calculations, and that is what we advocate in the present work. However, the quantitative impact of self-interaction and self-pairing processes on observable as well as the technical difficulties associated with their removal remain to be studied. As they do not lead to dramatic consequences, i.e., divergences and steps, this can be postponed.

As the proposed procedure must be implemented for all pairs of vacua involved in the multi reference calculation, the correction increases the basic computation cost. On the other hand, the number of summations in the calculation of the MR energy is significantly reduced in the canonical basis extracted to remove the spurious contributions. Thus, it might be of interest to take advantage of that fact in actual implementations of the MR-EDF formalism. This is the goal of a forthcoming publication to discuss such an implementation. In the meantime, another publication is devoted to illustrating the features of the correction method proposed in the present article by applying it to the rather transparent case of PNR [28].

Despite the success of regularized MR-EDF calculations documented in Ref. [28], some important questions remain unanswered as of today regarding the foundation and the implementation of MR methods within a consistent EDF framework. First, it is unclear in which sense the "projected" functional that one manipulates in such calculations can be attributed, at least implicitly, to a state belonging to a specific irreducible representation of the symmetry group of the nuclear Hamiltonian. The latter statement may seem rather paradoxical as the main purpose of those calculations is precisely to "restore the symmetries." The crucial point is that, as opposed to the *strict* projected Hartree-Fock-Bogoliubov approach [34–36], the MR energy functional is not obtained as the average value of a Hamiltonian in the projected state but as a functional of (nonobservable) transition densities defined for each pair of vacua belonging to the MR set. The rather complicated dependence on those densities and the use of different effective vertices (interactions) in different channels of the functional forbid the explicit refactorization of the energy in terms of the projected state. The benefit of such a method is that correlations that go beyond the strict projected-GCM approximation can be easily incorporated into the MR formalism. Again, the drawback is that it is not clear in which sense symmetries are actually restored in existing MR-EDF calculations. The clarification of such a question

and the proper formulation of symmetry restoration within a well-defined MR-EDF theory is mandatory in the near future.

Last but not least, the present work raises three important questions; the first two being related to the construction of energy density functionals; i.e., Skyrme, Gogny or any other types of realistic functionals.

(i) Only the removal of the most dangerous spurious terms associated with the use of the GWT as a basis to construct phenomenological MR energy kernels has been advocated in the present article and implemented in Ref. [28]. However, it is worth noting that SR- and MR-EDF calculations are also plagued with less dangerous pathologies related to *self-interaction* [89] and *self-pairing* [28]. In particular, such pathologies contaminate MR energy kernels independently on whether the SWT or the GWT is used as a basis to define them. At this point, though, we do not advocate the correction for self-interaction and self-pairing processes briefly discussed in the present article. The reason is that such additional corrections will impact explicitly the SR functional on which the MR calculation is based. This means that self-interaction- and self-pairing-free SR functionals must be constructed to test the importance of such spurious processes. This is a nontrivial step to take because doing so will modify the structure of usual functionals and most importantly the way self-consistent SR calculations usually work [89]. Such a work is underway.

(ii) The correction method proposed in the present work is based on using the Hamiltonian/wave-function framework, together with the SWT [41], as a reference point. A nontrivial implication is that the procedure provides a way to correct functionals that depends only on *integer* powers of the normal and anomalous density matrices [29]. As we do not see at this point how to proceed otherwise, the present work acts as a strong motivation to construct SR functionals that only involve integer powers of the density matrices in the near future. For reasons that are well known to practitioners, functionals depending on the third power in the local density do not work well enough and it remains to be seen whether using fourth powers of the local density is sufficient to construct high-precision energy density functionals.

(iii) The present work is a satisfactory solution to an extreme problem faced by MR energy density functional calculations. However, it is not entirely satisfying from a fundamental point of view because it amounts to correcting a phenomenological construction of multi reference energy kernels that is ill defined in the first place. Combined with related issues regarding restoration of symmetries, the present work calls for formal developments toward the derivation of a MR-EDF formalism from first principles. In particular, the regularization of the energy kernels happens to be basis dependent, just as standard self-interaction correction methods in DFT are [89]. A nice feature of the practical method we use to proceed to the regularization is that

it leads to a unique basis among all possible ones. It is so because, given $|\Phi_0\rangle$ and $|\Phi_1\rangle$, the application of the BMZ decomposition defines a unique basis, independently on the actual representation of the two states. Still, the fact that the removal of spurious contributions is basis dependent in the first place is not satisfactory and deserves some further attention in the future.

APPENDIX A: EXPRESSION OF $\langle\Phi_0|v_{123}|\Phi_1\rangle$

Using the method depicted in Sec. V B, we obtained the following expression:

$$
\begin{aligned}
\langle\Phi_0|\hat{v}_{123}|\Phi_1\rangle = {} & \frac{1}{6}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{V}_{m\mu}^{0*}\tilde{V}_{j\mu}^{0}V_{n\lambda}^{0*}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\langle\Phi_0|\Phi_1\rangle \\
& + \frac{1}{6}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{V}_{m\mu}^{0*}\tilde{V}_{j\mu}^{0}\tilde{U}_{n\bar{\lambda}}^{0}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\lambda\rangle \\
& + \frac{1}{6}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{U}_{m\bar{\mu}}^{0}\tilde{V}_{j\mu}^{0}V_{n\lambda}^{0*}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\mu}\mu}^{*}\langle\Phi_0|\Phi_1,\mu\rangle \\
& + \frac{1}{6}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{V}_{m\mu}^{0*}\tilde{V}_{j\mu}^{0}V_{n\lambda}^{0*}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\langle\Phi_0|\Phi_1,\nu\rangle \\
& + \frac{1}{6}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{U}_{m\bar{\mu}}^{0}\tilde{V}_{j\mu}^{0}V_{n\lambda}^{0*}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\bar{B}_{\bar{\mu}\mu}^{*}\langle\Phi_0|\Phi_1,\nu,\mu\rangle \\
& + \frac{1}{6}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{U}_{m\bar{\mu}}^{0}\tilde{V}_{j\mu}^{0}\tilde{U}_{n\bar{\lambda}}^{0}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\lambda}\lambda}^{*}\bar{B}_{\bar{\mu}\mu}^{*}\langle\Phi_0|\Phi_1,\mu,\lambda\rangle \\
& + \frac{1}{6}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{V}_{m\mu}^{0*}\tilde{V}_{j\mu}^{0}\tilde{U}_{n\bar{\lambda}}^{0}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\nu,\lambda\rangle \\
& + \frac{1}{6}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{U}_{m\bar{\mu}}^{0}\tilde{V}_{j\mu}^{0}\tilde{U}_{n\bar{\lambda}}^{0}\tilde{V}_{k\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\bar{B}_{\bar{\mu}\mu}^{*}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\nu,\mu,\lambda\rangle \\
& + \frac{1}{4}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{U}_{k\mu}^{0*}\tilde{V}_{m\lambda}^{0*}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\langle\Phi_0|\Phi_1\rangle \\
& + \frac{1}{4}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{U}_{k\mu}^{0*}\tilde{U}_{m\bar{\lambda}}^{0}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\lambda\rangle \\
& + \frac{1}{4}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{V}_{k\bar{\mu}}^{0}\tilde{V}_{m\lambda}^{0*}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\mu}\mu}^{*}\langle\Phi_0|\Phi_1,\mu\rangle \\
& + \frac{1}{4}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{U}_{k\mu}^{0*}\tilde{V}_{m\lambda}^{0*}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\langle\Phi_0|\Phi_1,\nu\rangle \\
& + \frac{1}{4}\sum \tilde{V}_{l\nu}^{0*}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{V}_{k\bar{\mu}}^{0}\tilde{U}_{m\bar{\lambda}}^{0}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\mu}\mu}^{*}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\mu,\lambda\rangle \\
& + \frac{1}{4}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{U}_{k\mu}^{0*}\tilde{U}_{m\bar{\lambda}}^{0}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\nu,\lambda\rangle \\
& + \frac{1}{4}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{V}_{k\bar{\mu}}^{0}\tilde{V}_{m\lambda}^{0*}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\bar{B}_{\bar{\mu}\mu}^{*}\langle\Phi_0|\Phi_1,\nu,\mu\rangle \\
& + \frac{1}{4}\sum \tilde{U}_{l\bar{\nu}}^{0}\tilde{V}_{i\nu}^{0}\tilde{V}_{j\mu}^{0}\tilde{V}_{k\bar{\mu}}^{0}\tilde{U}_{m\bar{\lambda}}^{0}\tilde{U}_{n\lambda}^{0}\bar{v}_{ijklmn}\bar{B}_{\bar{\nu}\nu}^{*}\bar{B}_{\bar{\mu}\mu}^{*}\bar{B}_{\bar{\lambda}\lambda}^{*}\langle\Phi_0|\Phi_1,\nu,\mu,\lambda\rangle,
\end{aligned} \tag{A1}
$$

where the sums run over all the indices, with the convention that when two or more ν_i's belong to the same conjugated pair, $\langle\Phi_0|\Phi_1,\nu_1,\cdots,\nu_n\rangle = 0$. In the latter expression, the first eight terms come from the expansion of $\rho^{01}\rho^{01}\rho^{01}$. Among these

terms, the four last ones will provide spurious contributions to $\mathcal{E}_{\mathrm{GWT}}^{\rho\rho\rho}$. Similarly, the remaining eight terms originate from $\rho^{01}\kappa^{10^*}\kappa^{01}$, whereas the last four of them provide spurious contribution to $\mathcal{E}_{\mathrm{GWT}}^{\rho\kappa\kappa}$.

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