Restoring broken symmetries for nuclei and reaction fragments

Aurel Bulgac

Phys. Rev. C **104**, 054601 — Published 1 November 2021

DOI: 10.1103/PhysRevC.104.054601

Restoring Broken Symmetries for Nuclei and Reaction Fragments

Aurel Bulgac[1, *]

[1] *Department of Physics, University of Washington, Seattle, Washington 98195–1560, USA*

In typical microscopic approaches, particularly when pairing correlations are present, nuclei and nuclear fragments do not have well defined quantum numbers and symmetries should be restored. I present here a formalism for the simultaneous projection of total particle numbers of a nucleus, particle number of reaction fragments, and of the reaction fragment intrinsic spins and of their correlation, and also for their symmetry restored densities and total energies. These new formulas for the symmetry restored quantities, are free of any singularities, unlike those in the previously introduced prescriptions.

I. INTRODUCTION

The problem of restoring broken symmetries within mean field treatments of nuclear systems is decades old, see monograph [1] and older references therein, and new studies are published on an almost constant pace over the years, see many references to more recent studies [2–8]. Essentially all studies published so far treat the case of either a Hartree-Fock (HF) or a Hartree-Fock-Bogoliubov (HFB) type of generalized Slater determinant. Such a generalized Slater determinant is typically used to minimize the total energy of a nucleus, either before or after minimization, within a mean field approach and from that procedure one extracts the restored symmetry nucleus wave functions.

This symmetry restored wave function in either static or time-dependent formulation of the framework is of the typical Generator Coordinate Method [9–12]. With the emergence of the Density Functional Theory (DFT) however, the role of the (generalized) Slater determinant was replaced by the (generalized) number densities, in which case the nuclear energy density functionals (NEDF) is not defined as an expectation value of a many-body Hamiltonian, but as an expectation of an energy density functional, which depends on several one-body densities. Trying to apply the HF(B) projection techniques to DFT studies leads to a number of difficulties. Some of these difficulties are discussed in Refs. [2–8].

The approach discussed here is based entirely on a treatment of strongly interacting many-fermion systems within the DFT framework, see Refs. [13–16] and references therein. The restoration of broken symmetries in case of DFT was discussed earlier [16] and it will be discussed in detail in this paper. The physical justification of such an approach was discussed earlier in Ref. [17], where a quantization of a semi-classical level was suggested, which can be easily converted into the projection technique discussed here. Unlike the approaches based on the generalized Wick theorem applied to generalized Slater determinants and evaluation of the total energy, the present approach is free of singularities, see Section VII. A few of the results discussed here have been briefly discussed in Ref. [16] and a few inaccuracies in that paper are corrected here.

This is a formal paper, where I derive a series of new formulas, not discussed previously in literature, needed in order to restore particle and rotation broken symmetries. In Section II I review some needed known facts. In Section III I describe how to double project the total number and the reaction fragment particle number for a reaction fragment. in Section IV I describe how to construct particle projected number and anomalous densities. In Sections V and VI I show how to simplify the particle projection in the canonical basis. In Section VI I present formulas for number and anomalous densities and for the number projected total energy. In Section VII I describe how to simultaneously project the total particle number and the particle number of a reaction fragment. In Section IX I develop formulas for double projection of the total and fragment number density. In Section X I show how to project the total particle and reaction fragment particle along with the intrinsic spins of the fragments and their correlations. The particular case of total and fragment particle numbers, the intrinsic fragment spins, and the total relative orbital momentum are discussed in Section XI. The last Section XII is devoted to the discussion of some numerical aspects. A number of formulas discussed here have been recently used in Refs. [18, 19].

These formulas presented here were developed for fission applications, but they can be used for heavy-ion reactions as well, with some small adjustments. The presentation here is restricted to systems with even particle parity, but its extension appears to be simple.

II. STRUCTURE OF A GENERALIZED SLATER DETERMINANT

The creation and annihilation quasi-particle operators are represented as [1]

$$\alpha_k^\dagger = \int d\xi \left[\mathrm{u}_k(\xi)\psi^\dagger(\xi) + \mathrm{v}_k(\xi)\psi(\xi) \right], \tag{1}$$

$$\alpha_k = \int d\xi \left[\mathrm{v}_k^*(\xi)\psi^\dagger(\xi) + \mathrm{u}_k^*(\xi)\psi(\xi) \right], \tag{2}$$

* bulgac@uw.edu

and the reverse relations

$$\psi^\dagger(\xi) = \sum_k \left[\mathrm{u}_k^*(\xi)\alpha_k^\dagger + \mathrm{v}_k(\xi)\alpha_k \right], \tag{3}$$

$$\psi(\xi) = \sum_k \left[\mathrm{v}_k^*(\xi)\alpha_k^\dagger + \mathrm{u}_k(\xi)\alpha_k \right], \tag{4}$$

where $\psi^\dagger(\xi)$ and $\psi(\xi)$ are the field operators for the creation and annihilation of a particle with coordinate ξ. The normal number (Hermitian $n = n^\dagger$) and anomalous (skew symmetric $\kappa = -\kappa^T$) densities are

$$\begin{aligned} n(\xi,\xi') &= \langle\Phi|\psi^\dagger(\xi')\psi(\xi)|\Phi\rangle \\ &= \sum_k \mathrm{v}_k^*(\xi)\mathrm{v}_k(\xi') = \sum_{l=n,\bar{n}} v_l^2 \phi_l^*(\xi)\phi_l(\xi'), \end{aligned} \tag{5}$$

$$\begin{aligned} \kappa(\xi,\xi') &= \langle\Phi|\psi(\xi')\psi(\xi)|\Phi\rangle \\ &= \sum_k \mathrm{v}_k^*(\xi)\mathrm{u}_k(\xi') = \sum_{l=n,\bar{n}} u_l v_l \phi_l^*(\xi)\phi_{\bar{l}}^*(\xi'), \end{aligned} \tag{6}$$

$$\int d\xi \phi_k^*(\xi)\phi_l(\xi) = \delta_{kl}, \tag{7}$$

with $u_l^2 + v_l^2 = 1$, $0 \le u_l = u_{\bar{l}} \le 1$, $0 \le v_l = -v_{\bar{l}} \le 1$, and n and $\bar{n}$ denote time-reversed states in the canonical representation [1, 20, 21], and where

$$\alpha_k|\Phi\rangle = 0, \quad |\Phi\rangle = \mathcal{N}\prod_k \alpha_k|0\rangle, \quad \langle\Phi|\alpha_k\alpha_l^\dagger|\Phi\rangle = \delta_{kl}, \tag{8}$$

where $\mathcal{N}$ is a normalization factor, determined up to an arbitrary phase, and assuming that $\alpha_k|0\rangle \ne 0$ for any k. In case any $\int d\xi|\mathrm{v}_k(\xi)|^2 = 0$ or $\alpha_k|0\rangle = 0$ the corresponding factor α_k is skipped. Here the discussion will be explicitly limited to systems with an even particle number parity, as the extension to the general case is trivial [1].

Here I will elaborate at first on details of the projection technique developed in Ref. [16], which were not discussed before. The particle projection on a fragment of the system is performed with the help of the unitary operator, introduced earlier in Ref. [22]

$$\hat{P}^\Theta(\eta) = e^{i\eta\int d\xi \Theta(\xi)\psi^\dagger(\xi)\psi(\xi)} = e^{i\eta\hat{N}^\Theta}, \tag{9}$$

$$\hat{N}^\Theta = \int d\xi \Psi^\dagger(\xi)\psi(\xi)\Theta(\xi), \tag{10}$$

$$\Theta^2(\xi) = \Theta(\xi), \quad \hat{P}^\Theta(\eta)\hat{P}^\Theta(-\eta) = 1, \quad \eta \in [-\pi,\pi] \tag{11}$$

$\Theta(\xi)$ is the Heaviside function and for all non-negative integer particle numbers

$$|\Phi^\Theta(N)\rangle = \int_{-\pi}^{\pi} \frac{d\eta}{2\pi} e^{-i\eta N}\hat{P}^\Theta(\eta)|\Phi\rangle. \tag{12}$$

is the component of the wave function $|\Phi\rangle$ with exactly N particles in the space region where $\Theta(\xi) = 1$.

One can easily show that under the transformation with this operator the field and quasiparticle operators change according to the rules

$$\begin{aligned} \psi^\dagger(\xi,\eta) &= \hat{P}^\Theta(\eta)\psi^\dagger(\xi)\hat{P}^\Theta(-\eta) = e^{i\eta\Theta(\xi)}\psi^\dagger(\xi), \\ \tilde{\alpha}_k(\eta) &= \int d\xi \left[e^{i\eta\Theta(\xi)}\mathrm{v}_k^*(\xi)\psi^\dagger(\xi) + e^{-i\eta\Theta(\xi)}\mathrm{u}_k^*(\xi)\psi(\xi) \right]. \end{aligned} \tag{13}$$

It is easy to show that

$$\{\tilde{\alpha}_k^\dagger(\eta), \tilde{\alpha}_l(\eta)\} = \delta_{kl}, \quad \{\tilde{\alpha}_k(\eta), \tilde{\alpha}_l(\eta)\} = 0. \tag{14}$$

This implies that when $\Theta(\xi) \equiv 1$ the components of the quasiparticle wave functions (qpwfs) change as

$$[\mathrm{v}_k^*(\xi), \mathrm{u}_k^*(\xi)] \to [e^{i\eta\Theta(\xi)}\mathrm{v}_k^*(\xi), e^{-i\eta\Theta(\xi)}\mathrm{u}_k^*(\xi)]. \tag{15}$$

and correspondingly the new vacuum is (assuming that for all $\tilde{\alpha}_k|0\rangle > 0$)

$$|\tilde{\Phi}(\eta)\rangle = \mathcal{N}\prod_k \tilde{\alpha}_k(\eta)|0\rangle = \hat{P}^\Theta(\eta)|\Phi\rangle. \tag{16}$$

In the case $2\Omega = 4$ the wave function $|\Phi\rangle$ will have 4-particle, 2-particle, and 0-particle components. A typical 2-particle component arising from

$$\int d\xi_1 d\xi_2 d\xi_3 d\xi_4 \; \mathrm{u}_1^*(\xi_1)\mathrm{v}_2^*(\xi_2)\mathrm{v}_3^*(\xi_3)\mathrm{v}_4^*(\xi_4) \\ \psi(\xi_1)\psi^\dagger(\xi_2)\psi^\dagger(\xi_3)\psi^\dagger(\xi_4)|0\rangle$$

has the structure

$$\begin{aligned} &= \int d\xi \mathrm{u}_1^*(\xi)\mathrm{v}_2^*(\xi) \int d\xi_1 d\xi_2 \mathrm{v}_3^*(\xi_1)\mathrm{v}_4^*(\xi_2)\psi^\dagger(\xi_1)\psi^\dagger(\xi_2)|0\rangle \\ &- \int d\xi \mathrm{u}_1^*(\xi)\mathrm{v}_3^*(\xi) \int d\xi_1 d\xi_2 \mathrm{v}_2^*(\xi_1)\mathrm{v}_4^*(\xi_2)\psi^\dagger(\xi_1)\psi^\dagger(\xi_2)|0\rangle \\ &+ \int d\xi \mathrm{u}_1^*(\xi)\mathrm{v}_4^*(\xi) \int d\xi_1 d\xi_2 \mathrm{v}_1^*(\xi_1)\mathrm{v}_4^*(\xi_2)\psi^\dagger(\xi_1)\psi^\dagger(\xi_2)|0\rangle. \end{aligned}$$

There are two more contributions to the 2-particle component arising from the terms containing the combinations of field operators $\psi^\dagger(\xi_1)\psi(\xi_2)\psi^\dagger(\xi_3)\psi^\dagger(\xi_4)$ and $\psi^\dagger(\xi_1)\psi^\dagger(\xi_2)\psi(\xi_3)\psi^\dagger(\xi_4)$.

After applying the operator $\hat{P}^\Theta(\eta)$ on the above 2-particle component only the quasiparticle v-components change as $\mathrm{v}_k^*(\xi) \to e^{i\eta\Theta(\xi)}\mathrm{v}_k^*(\xi)$, but only for terms with factors like $\int d\xi \mathrm{v}_k(\xi)\psi^\dagger(\xi)$. Terms containing factors of the type $\int d\xi \mathrm{u}_k(\xi)\psi(\xi)$ do not survive after normal ordering. The terms like $\int d\xi \mathrm{u}_k^*(\xi)\mathrm{v}_l^*(\xi)$ are left invariant by either by transformation Eq. (15) or by the operator $\hat{P}^\Theta(\eta)$.

According to the analysis performed above on the example of $2\Omega = 4$ only the overlaps between the v-components of the qpwfs in the Onishi-Yoshida [1, 23] formula are changed, namely

$$\begin{aligned} \langle\Phi|\hat{P}^\Theta(\eta)|\Phi\rangle &= \sqrt{\det\left[\langle \mathrm{u}_k|\mathrm{u}_l\rangle + \langle \mathrm{v}_k|e^{i\eta\Theta}|\mathrm{v}_l\rangle\right]} \\ &= \sqrt{\det\left[\delta_{kl} + (e^{i\eta} - 1)\langle \mathrm{v}_k|\Theta|\mathrm{v}_l\rangle\right]}. \end{aligned} \tag{17}$$

One should note, that no overlaps of the type $\int d\xi \mathrm{u}_k^*(\xi)\mathrm{v}_l^*(\xi)\Theta(\xi)$ appear in the Onishi-Yoshida overlap formula, which otherwise might have led to spurious terms.

III. DOUBLE PROJECTION OF FRAGMENT PARTICLE NUMBER AND ALSO OVERALL PARTICLE NUMBER

When evaluating the particle number of a fragment one should remember that its particle number distribution is affected by the uncertainty in the particle number in the total many-body wave function. Let me consider the projection of the total particle number

$$e^{i\eta_0 \hat{N}}|\Phi\rangle = \sum_{n=0}^{\Omega} a_{2n} e^{2in\eta_0}|\Phi_{2n}\rangle, \tag{18}$$

$$\sum_{n=0}^{\Omega} |a_{2n}|^2 = 1, \quad \hat{N} = \int d\xi \psi^\dagger(\xi)\psi(\xi), \tag{19}$$

where $n = N$ are non-negative integers and Φ_{2n} are linear combinations of ordinary Slater determinants for exactly $N = 2n$ particles. Since only even $2n\eta_0$ frequencies are present one can limit the integral over the interval $\eta_0 \in [-\pi/2, \pi/2]$.

The wave function (16) constructed for $\Theta \equiv 1$

$$|\tilde{\Phi}(\eta_0)\rangle = \hat{P}^\Theta(\eta_0)|\Phi\rangle = \mathcal{N} \prod_k \tilde{\alpha}_k(\eta_0)|0\rangle, \tag{20}$$

with the operators

$$\tilde{\alpha}_k(\eta_0) = \int d\xi \left[e^{i\eta_0} \mathrm{v}_k^*(\xi)\psi^\dagger(\xi) + e^{-i\eta_0}\mathrm{u}_k^*(\xi)\psi(\xi)\right]. \tag{21}$$

has according to Onishi-Yoshida formula the overlap

$$\langle\Phi|\tilde{\Phi}(\eta_0)\rangle = \sqrt{\det\left[e^{-i\eta_0}\langle \mathrm{u}_k|\mathrm{u}_l\rangle + e^{i\eta_0}\langle \mathrm{v}_k|\mathrm{v}_l\rangle\right]}, \tag{22}$$

$$= e^{-i\eta_0\Omega}\sqrt{\det\left[\delta_{kl} + (e^{2i\eta_0} - 1)\langle \mathrm{v}_k|\mathrm{v}_l\rangle\right]} \tag{23}$$

with both positive and negative frequencies $e^{in\eta_0}$,

$$\langle\Phi|\tilde{\Phi}(\eta_0)\rangle = e^{-i\eta_0\Omega}\sum_{m=0}^{2\Omega} \tilde{a}_{2m} e^{2im\eta_0}. \tag{24}$$

From the arguments presented in Sections V and VI and from our numerical simulations as well it follows that the frequency spectrum lies in the interval $[-\Omega, \Omega]\eta_0$, unlike the natural expansion Eq. (18), where only the expected terms with $0 \le N = 2n \le 2\Omega$ are present. In the particular case of ordinary Slater determinant with exactly N-particles one obtains using Onishi-Yoshida formula

$$\langle\Phi|\tilde{\Phi}(\eta_0)\rangle = e^{-i\eta_0\Omega} e^{i\eta_0 N}, \tag{25}$$

since $\langle \mathrm{u}_k|\mathrm{u}_k\rangle + \langle \mathrm{v}_k|\mathrm{v}_k\rangle = 1$ and there are exactly N overlaps $\langle \mathrm{v}_k|\mathrm{v}_k\rangle = 1$, while the rest $2\Omega - N$ such overlaps vanish. Thus, using Onishi-Yoshida overlap formula results in an incorrect frequency spectrum, a situation which can be quite easily rectified as suggested below.

It is useful to introduce a different set of annihilation operators [16]

$$\alpha_k(\eta_0) = \int d\xi [e^{2i\eta_0}\mathrm{v}_k^*(\xi)\psi^\dagger(\xi) + \mathrm{u}_k(\xi)\psi(\xi)] \tag{26}$$

$$= e^{-i\eta_0}\tilde{\alpha}_k(\eta_0) = \sum_l [A_{kl}(\eta_0)\alpha_l + B_{kl}(\eta_0)\alpha_l^\dagger], \tag{27}$$

$$A_{kl}(\eta_0) = \delta_{kl} + (e^{2i\eta_0} - 1)\int d\xi \mathrm{v}_k^*(\xi)\mathrm{v}_l(\xi) \tag{28}$$

$$B_{kl}(\eta_0) = (e^{2i\eta_0} - 1)\int d\xi \mathrm{v}_k^*(\xi)\mathrm{u}_l^*(\xi), \tag{29}$$

with the new associated qpwfs

$$[\mathrm{v}_k^*(\xi), \mathrm{u}_k^*(\xi)] \to [e^{i2\eta_0}\mathrm{v}_k^*(\xi), \mathrm{u}_k^*(\xi)] \tag{30}$$

and

$$|\Phi(\eta_0)\rangle = \mathcal{N}\prod_k \alpha_k(\eta_0)|0\rangle. \tag{31}$$

On can then easily see that

$$\langle\Phi|\Phi(\eta_0)\rangle = e^{i\eta_0\Omega}\langle\Phi|\tilde{\Phi}(\eta_0)\rangle = \sum_{n=0}^{\Omega} a_{2n}e^{2in\eta_0}, \tag{32}$$

similarly to Eq. (18) and also that

$$\langle\Phi|\Phi(\eta_0)\rangle = e^{i\eta_0 N} \tag{33}$$

for the case of an ordinary Slater determinant for N-particles one obtains the correct result. These conclusions are also confirmed in Sections V and VI, where an analysis is performed using the canonical basis. Numerical simulations also show that $\max_N |a_N|^2$ occurs, as naturally expected, for $N \approx \langle\Phi|\hat{N}|\Phi\rangle$, see also Ref. [16].

It then follows that the projected overlap on the total particle number N wave function

$$\langle\Phi|\Phi_N(\eta^{\mathrm{F}})\rangle = \int_{-\pi}^{\pi}\frac{d\eta_0}{2\pi}e^{-i\eta_0 N}\langle\Phi|\Phi(\eta_0, \eta^{\mathrm{F}})\rangle, \tag{34}$$

$$\langle\Phi|\Phi(\eta_0, \eta^{\mathrm{F}})\rangle = \mathcal{N}(\eta_0, \eta^{\mathrm{F}}) \tag{35}$$

$$\times \langle\Phi|\prod_k \int d\xi \left[e^{2i\eta_0}e^{i\eta^{\mathrm{F}}\Theta^{\mathrm{F}}(\xi)}\mathrm{v}_k^*(\xi)\psi^\dagger(\xi) + \mathrm{u}_k^*(\xi)\psi(\xi)\right]|0\rangle$$

is a sum of overlaps of (ordinary) Slater determinants for exactly N-particles, where $0 \le N \le 2\Omega$ is even.

As I discussed in the previous section, in $|\Phi\rangle = \mathcal{N}\prod_{k=1}^{2\Omega}\alpha_k|0\rangle$ only terms with an even number creation operators $\psi^\dagger(\xi)$ and no annihilation operators $\psi(\xi)$ survive after normal ordering. The integration over the angle η_0 selects only terms with exactly N creation operators $\psi^\dagger(\xi)$ from $|\Phi(\eta_0, \eta^{\mathrm{F}})\rangle$. In order to correctly evaluate the particle number in a reaction fragment one has to perform a double particle number projection, on the total particle number N and on the fragment particle (integer) number N^{F}, where $0 \le N^{\mathrm{F}} \le N$.

In order to accurately determine the particle number in a fission fragment (FF) one has to perform a double particle projection [24–26], the first projection to fix the total particle number in the fissioning nucleus and the second projection to determine the particle number in the FF. One has thus to consider the overlap

$$\langle\Psi|\Psi(\eta_0,\eta^{\rm F})\rangle = \sqrt{\det\left[\delta_{kl} + \langle {\rm v}_k|e^{2i\eta_0}e^{i\eta^{\rm F}\Theta^{\rm F}} - 1|{\rm v}_l\rangle\right]}$$

$$= \sqrt{\det\left[\delta_{kl} + (e^{2i\eta_0}-1)O_{kl} + e^{2i\eta_0}(e^{i\eta^{\rm F}}-1)O^{\rm F}_{kl}\right]}, \quad (36)$$

$$O_{kl} = \langle {\rm v}_k|{\rm v}_l\rangle, \quad O^{\rm F}_{kl} = \langle {\rm v}_k|\Theta^{\rm L,H}|{\rm v}_l\rangle, \quad (37)$$

$$O^{\rm H}_{kl} + O^{\rm L}_{kl} = O_{kl}, \quad \text{if} \quad \Theta^{\rm L} + \Theta^{\rm H} = 1, \quad (38)$$

and where $\Theta^{\rm F} = \Theta^{\rm L,H}$ selects the spatial region of either the heavy (H) or of the light (L) FF. The double particle projection is required as the initial state does not have a well defined particle number. Since $N = N^{\rm L} + N^{\rm H}$ the probability distributions for the two FFs are related $P(N, N^{\rm L}) = P(N, N - N^{\rm H})$, where

$$P(N,N^{\rm F}) = 2\int_0^{\pi/2}\frac{d\eta_0}{\pi}\int_0^{\pi}\frac{d\eta^{\rm F}}{\pi} \times {\rm Re}\left[\langle\Psi|\Psi(\eta_0,\eta^{\rm F})\rangle e^{-i\eta_0 N - i\eta^{\rm F}N^{\rm F}}\right] \quad (39)$$

For systems with even particle number N one can restrict $\eta_0 \in [-\pi/2, \pi/2]$. The particle probability distribution in a fragment is given by the conditional probability

$$P_N(N^{\rm F}) = \frac{P(N,N^{\rm F})}{\sum_{N^{\rm F}=0}^{N} P(N,N^{\rm F})}. \quad (40)$$

In case of a reaction between two superfluid nuclei one needs to perform a triple projection, on both initial partners and one on the final fragment.

The attentive reader has noticed that in Ref. [16] it was argued that for a FF particle projection, where the projection on the total particle number was not considered, one should use the overlap

$$\langle\Psi|\Psi(\eta^{\rm F})\rangle = \sqrt{\det\left[\delta_{kl} + \langle {\rm v}_k|e^{i\eta^{\rm F}\Theta^{\rm F}} - 1|{\rm v}_l\rangle\right]}$$

$$= \sqrt{\det\left[\delta_{kl} + (e^{i\eta^{\rm F}}-1)O^{\rm F}_{kl}\right]}. \quad (41)$$

Since the projection on the total particle number selects in Eq. (36) overlaps of ordinary Slater determinants, the projection of the FF particle number can proceed following the procedure outlined above, see Eqs. (34) and (35), as it was established earlier in the literature [16, 22].

IV. PROJECTING THE PARTICLE NUMBER FOR AN ARBITRARY ONE-BODY OBSERVABLE

Here I will derive a formula for a particle average of the operator $\hat{Q} = \int d\xi d\xi' \langle\xi|Q|\xi'\rangle\psi^\dagger(\xi)\psi(\xi')$. Consider at first the transformation

$$\mathrm{u}_k(\xi,\epsilon) = \mathrm{u}_k(\xi), \quad \mathrm{v}_k(\xi,\epsilon) = e^{2\epsilon\hat{Q}}\mathrm{v}_k(\xi), \quad (42)$$

one can show that

$$\left.\frac{d\langle\Phi|\Phi(\epsilon)\rangle}{d\epsilon}\right|_{\epsilon=0} = \lim_{\epsilon\to 0}\frac{\sqrt{\det\left[\delta_{kl} + \langle {\rm v}_k|e^{2\epsilon\hat{Q}} - 1|{\rm v}_l\rangle\right]}}{\epsilon}$$

$$= \sum_k \langle {\rm v}_k|\hat{Q}|{\rm v}_k\rangle = \langle\Phi|\hat{Q}|\Phi\rangle, \quad (43)$$

where $|\Phi(\epsilon)\rangle$ was constructed with qpwfs (42). Since one needs the "deformed" quasi-particle wave functions with an accuracy $\mathcal{O}(\epsilon)$ only one can use $1+2\epsilon\hat{Q}$ instead of $e^{2\epsilon\hat{Q}}$. In this case the transformation of the quasi-particle wave functions is

$$\mathrm{u}_n(\xi,\epsilon) = \mathrm{u}_n(\xi), \quad (44)$$

$$\mathrm{v}_n(\xi,\epsilon) = \int d\xi'[\delta(\xi-\xi') + 2\epsilon\langle\xi|Q|\xi'\rangle]\mathrm{v}_n(\xi').$$

The number density matrix - and in a similar manner the anomalous density, see below - is naturally defined as a functional derivative, see Negele and Orland [27] and Furnstahl [28],

$$n(\xi,\xi') = \frac{\delta q}{\delta\langle\xi|Q|\xi'\rangle}, \text{ where } q = \langle\Phi|\hat{Q}|\Phi\rangle \quad (45)$$

This definition of the number density matrix, as the functional derivative of the partition function with respect to an arbitrary external field and which widely used in quantum field theory for decades, is the main difference between the broken symmetry restoration framework described here and those introduced in previous approaches. The density matrix is thus naturally defined as the response or the measurement due to an appropriately chosen weak external probe acting on the system.

The normal particle projected one-body density can be calculated as the variational derivative

$$n(\xi,\xi'|\eta_0) = \frac{\delta q(\eta_0)}{\delta\langle\xi|Q|\xi'\rangle} \quad (46)$$

where, in order to evaluate $q(\eta_0)$ one should use now the overlap

$$\langle\Phi|\Phi(\epsilon,\eta_0)\rangle = \sqrt{\det\left[\delta_{kl} + \langle {\rm v}_k|e^{2i\eta_0}e^{2\epsilon\hat{Q}} - 1|{\rm v}_l\rangle\right]} \quad (47)$$

and thus

$$n(\xi,\xi'|\eta_0) = \langle\Phi|\Phi(\eta_0)\rangle e^{2i\eta_0}\sum_{kl}{\rm v}^*_k(\xi){\rm v}_l(\xi')\,a_{lk}(\eta_0). \quad (48)$$

The matrix $a_{kl}(\eta_0)$ is the inverse of the matrix $A_{kl}(\eta_0)$

$$A_{kl}(\eta_0) = [\delta_{kl} + (e^{2i\eta_0}-1)\langle {\rm v}_k|{\rm v}_l\rangle], \quad (49)$$

$$\sum_l A_{kl}(\eta_0)a_{lm}(\eta_0) = \delta_{km}. \quad (50)$$

In the case of the anomalous density $\kappa(\xi,\xi'|\eta_0)$ one would have to consider a transformation different from Eq. (97), namely the transformation

$$u_n(\xi,\epsilon,\eta_0) = u_n(\xi) + 2\epsilon\int d\xi'\langle\xi|\Delta|\xi'\rangle e^{2i\eta_0}v_n(\xi'),$$

$$v_n(\xi,\epsilon,\eta_0) = v_n(\xi) \quad (51)$$

in order to construct $|\Phi(\epsilon,\eta_0)\rangle$ and follow the same steps as in the case of a normal operator $\hat{Q}$ outlined above and obtain for the anomalous density Eq. (6)

$$\kappa(\xi,\xi'|\eta_0) = \langle\Phi|\Phi(\eta_0)\rangle e^{2i\eta_0}\sum_{lk}\mathrm{v}_k^*(\xi)\mathrm{u}_l(\xi')\,a_{lk}(\eta_0). \quad (52)$$

These formulas simplify significantly in the canonical basis, see Section VI.

V. CANONICAL BASIS

The calculation of the particle projected averages are greatly simplified in the canonical basis. After diagonalizing the overlap $O_{kl} = \langle \mathrm{v}_k|\mathrm{v}_l\rangle$ of the v-components the new qpwfs satisfy the relations

$$\langle\tilde{\mathrm{v}}_k|\tilde{\mathrm{v}}_l\rangle = n_k\delta_{kl} \quad (53)$$

it follows that the overlap matrix of the u_k-components is also diagonal

$$\langle\tilde{\mathrm{u}}_k|\tilde{\mathrm{u}}_l\rangle = (1-n_k)\delta_{kl}, \quad (54)$$

and the average particle number is given by

$$N = \sum_k n_k. \quad (55)$$

The occupation probabilities $n_k = \langle\tilde{\mathrm{v}}_k|\tilde{\mathrm{v}}_k\rangle$ are different from $\langle\mathrm{v}_k|\mathrm{v}_k\rangle$, even though their sums add to the same total particle number N, due to invariance of the trace of a matrix. The number of v_k-components is $2\Omega = 2N_xN_yN_z$ for neutrons and protons respectively. In an infinite box $2\Omega=\infty$.

It is useful to introduce the unitary transformation, and correspondingly the set of eigenvectors, which diagonalizes O_{kl}

$$\sum_l O_{kl}\mathcal{U}_{lm} = \mathcal{U}_{km}n_m, \quad \sum_n \mathcal{U}^*_{km}\mathcal{U}_{kn} = \delta_{mn}, \quad (56)$$

$$\mathrm{v}_k(\xi) = \sum_m \mathcal{U}_{km}\tilde{\mathrm{v}}_m(\xi), \quad \tilde{\mathrm{v}}_n(\xi) = \sum_l \mathcal{U}^*_{ln}\mathrm{v}_l(\xi) \quad (57)$$

$$O_{kl} = \sum_m \mathcal{U}_{km}n_m\mathcal{U}^*_{lm}. \quad (58)$$

In the canonical basis the overlap for the double particle projection Eq. (36) acquire the simpler form

$$\langle\Psi|\Psi(\eta_0,\eta^{\mathrm{F}})\rangle \quad (59)$$
$$= \sqrt{\det\left[[1+(e^{2i\eta_0}-1)n_k]\delta_{kl} + e^{2i\eta_0}(e^{i\eta^{\mathrm{F}}}-1)\tilde{O}^{\mathrm{F}}_{kl}\right]},$$
$$\tilde{O}^{\mathrm{F}}_{kl} = \langle\tilde{\mathrm{v}}_k|\Theta^{\mathrm{L,H}}|\tilde{\mathrm{v}}_l\rangle. \quad (60)$$

The overlap $\langle\tilde{\mathrm{v}}_k(t)|\tilde{\mathrm{v}}_l(t)\rangle$ does not remain diagonal as a function of time in a time-dependent evolution. For that reason the simplified formulas for the number projected quantities should be derived in the canonical basis determined at the time when the corresponding observables are needed.

VI. TEXTBOOK DEFINITION OF THE CANONICAL BASIS

Since the eigenvalues of the matrix $\mathcal{O}_{kl}$ are double degenerate and can always choose the canonical qpwfs $\tilde{\mathrm{u}}_k(\xi), \tilde{\mathrm{v}}_k(\xi)$ of the textbook form [1]

$$|\Phi\rangle = \mathcal{N}\prod_{n=1}^{\Omega}\alpha_n\alpha_{\overline{n}}|0\rangle = \prod_{n=1}^{\Omega}(u_n + v_n a^\dagger_n a^\dagger_{\overline{n}})|0\rangle, \quad (61)$$

where

$$\alpha_n = u_n a_n - v_n a^\dagger_{\overline{n}}, \quad \alpha_{\overline{n}} = u_n a_{\overline{n}} + v_n a^\dagger_n, \quad (62)$$

$$a^\dagger_n = \int d\xi\phi_n(\xi)\psi^\dagger(\xi), \quad a^\dagger_{\overline{n}} = \int d\xi\phi_{\overline{n}}(\xi)\psi^\dagger(\xi), \quad (63)$$

$$\langle\phi_n|\phi_n\rangle = \langle\phi_{\overline{n}}|\phi_{\overline{n}}\rangle = 1, \quad \langle\phi_{\overline{n}}|\phi_n\rangle = 0 \quad (64)$$

and real $u_n\geq 0$, $v_n \geq 0$.

After normal ordering one obtains

$$\alpha_n\alpha_{\overline{n}} = v_n^2 a^\dagger_n a^\dagger_{\overline{n}} + u_nv_n \quad (65)$$
$$+ u_n^2 a_n a_{\overline{n}} - u_nv_n(a^\dagger_n a_n + a^\dagger_{\overline{n}}a_{\overline{n}}).$$
$$\frac{1}{v_n}\alpha_n\alpha_{\overline{n}}|0\rangle = (u_n + v_n a^\dagger_n a^\dagger_{\overline{n}})|0\rangle, \quad u_n^2+v_n^2 = 1. \quad (66)$$

After a gauge transformation $\hat{P}^{\Theta}(\eta)\,\alpha_n\alpha_{\overline{n}}|0\rangle$ only the creation operators $a^\dagger_n a^\dagger_{\overline{n}}$ in first term in Eq. (66) are affected by the action of $\hat{P}^{\Theta}(\eta)$. Then the overlap

$$\frac{1}{v_mv_n}\langle 0|\alpha^\dagger_{\overline{m}}\alpha^\dagger_m\,\hat{P}^{\Theta}(\eta)\,\alpha_n\alpha_{\overline{n}}|0\rangle$$
$$= u_mu_n + v_mv_n\langle 0|a_{\overline{m}}a_m\hat{P}^{\Theta}(\eta)a^\dagger_n a^\dagger_{\overline{n}}|0\rangle. \quad (67)$$

The matrix element can be simplified

$$\langle 0|a_{\overline{m}}a_m\hat{P}^{\Theta}(\eta)a^\dagger_n a^\dagger_{\overline{n}}|0\rangle = \quad (68)$$
$$= \{\ [\delta_{mn} + (e^{i\eta}-1)\langle\phi_m|\Theta|\phi_n\rangle]$$
$$\times[\delta_{mn} + (e^{i\eta}-1)\langle\phi_{\overline{m}}|\Theta|\phi_{\overline{n}}\rangle]$$
$$-(e^{i\eta}-1)^2\langle\phi_m|\Theta|\phi_{\overline{n}}\rangle\langle\phi_{\overline{m}}|\Theta|\phi_n\rangle\}.$$

If $\Theta(\xi)\equiv 1$ this formula simplifies

$$\frac{1}{v_mv_n}\langle 0|\alpha^\dagger_{\overline{m}}\alpha^\dagger_m\hat{P}^{\Theta}(\eta)\alpha_n\alpha_{\overline{n}}|0\rangle = \delta_{mn}[u_n^2 + e^{2i\eta}v_n^2]. \quad (69)$$

I will introduce now the gauge transformed operators and total wave function and using Eq. (66) one obtains

$$\alpha_n(\eta_0) = u_na_n - v_ne^{2i\eta_0}a^\dagger_{\overline{n}}, \quad (70)$$

$$\alpha_{\overline{n}}(\eta_0) = u_na_{\overline{n}} + v_ne^{2i\eta_0}a^\dagger_n, \quad (71)$$

$$\alpha_n|\Phi(\eta_0)\rangle = 0,\ \alpha_{\overline{n}}|\Phi(\eta_0\rangle = 0, \quad (72)$$

$$|\Phi(\eta_0)\rangle = \sum_{n=0}^{\Omega}a_{2n}e^{2i\eta_0 n}|\Phi_{2n}\rangle, \quad (73)$$

$$\sum_{n=0}^{\Omega}|a_{2n}|^2 = 1, \quad (74)$$

and where $n, \overline{n} = 1, \dots, \Omega$ and where $|\Phi_{2n}\rangle$ are sums of (ordinary) Slater determinants for exactly $N = 2n$ particles. The particle probability distribution is thus given by

$$P(N) = |a_N|^2 = 2\,\mathrm{Re}\int_0^{\pi/2}\frac{d\eta_0}{\pi}e^{-i\eta_0 N}\langle\Phi|\Phi(\eta_0)\rangle, \quad (75)$$

$$\langle\Phi|\Phi(\eta_0)\rangle = \prod_{n=1}^{\Omega}[u_n^2 + v_n^2 e^{2i\eta_0}], \quad (76)$$

where the integration integral was halved, since $\langle\Phi|\Phi(\eta_0+\pi)\rangle = \langle\Phi|\Phi(\eta_0)\rangle$.

In the case of double particle projection one introduces the quasiparticle operators

$$\alpha_n(\eta_0,\eta^{\mathrm{F}}) = -v_n e^{2i\eta_0}\int d\xi \phi_n(\xi)e^{i\eta^{\mathrm{F}}\Theta^{\mathrm{F}}(\xi)}\psi^\dagger(\xi) + u_n a_n, \quad (77)$$

$$\alpha_{\overline{n}}(\eta_0,\eta^{\mathrm{F}}) = v_n e^{2i\eta_0}\int d\xi \phi_{\overline{n}}(\xi)e^{i\eta^{\mathrm{F}}\Theta^{\mathrm{F}}(\xi)}\psi^\dagger(\xi) + u_n a_{\overline{n}}, \quad (78)$$

and the corresponding overlap has the structure

$$\langle\Phi|\Phi(\eta_0,\eta^{\mathrm{F}})\rangle = \sqrt{\det\left[\delta_{kl} + \mathrm{v}_k\mathrm{v}_l\langle\phi_k|e^{2i\eta_0}e^{i\eta^{\mathrm{F}}\Theta^{\mathrm{F}}} - 1|\phi_l\rangle\right]}, \quad (79)$$

where k, l run over both sets of $n, \overline{n} = 1, \dots, \Omega$ and $n_{k,l} = \mathrm{v}_{k,l}^2$ are occupation probabilities, see Eq. (53).

VII. PARTICLE NUMBER PROJECTED DENSITIES AND TOTAL ENERGY

For any FF observables expression of the projected densities are useful. The densities $n(\xi,\xi'|\eta_0)$, Eq. (48) and $\kappa(\xi,\xi'|\eta_0)$, Eq. (52) acquire in the canonical basis a simple form

$$n(\xi,\xi'|\eta_0) = \langle\Phi|\Phi(\eta_0)\rangle\sum_k\frac{\tilde{\mathrm{v}}_k^*(\xi)\tilde{\mathrm{v}}_k(\xi')e^{2i\eta_0}}{1+(e^{2i\eta_0}-1)n_k}, \quad (80)$$

$$\kappa(\xi,\xi'|\eta_0) = \langle\Phi|\Phi(\eta_0)\rangle\sum_k\frac{\tilde{\mathrm{v}}_k^*(\xi)\tilde{\mathrm{u}}_k(\xi')e^{2i\eta_0}}{1+(e^{2i\eta_0}-1)n_k}, \quad (81)$$

where the sum and products run over all quasiparticle states. The use of Eqs. (48) and 52 for the definition of the number and anomalous densities, as a functional derivative of the expectation value of an observable, is what distinguishes my approach from previous approaches in literature. One can easily show that in the canonical basis,

$$\langle\Phi|\Phi(\eta_0)\rangle = \prod_{k=1}^{2\Omega}\sqrt{1+(e^{2i\eta_0}-1)n_k} \quad (82)$$

and where the canonical occupation numbers n_k are double degenerate. For this reason there is no singularity in Eqs. (80) and (81) when $1+(e^{2i\eta_0}-1)n_k = 0$ only when both $\eta_0 = \pm\pi/2$ and $n_k = 1/2$. For $\eta = 0$ one obtains the corresponding unprojected densities. Formulas for projected densities on both the total and fragment numbers are straightforward to derive.

Notice that the qpwfs

$$\sum_k \mathrm{u}_k(\xi)\mathrm{u}_k^*(\xi') + \mathrm{v}_k(\xi)\mathrm{v}_k^*(\xi') = \delta(\xi-\xi') \quad (83)$$

form a complete non-orthogonal set. This holds true for the qpwfs in the canonical basis as well.

It is useful as well to define the projected density matrix respectively

$$n(\xi,\xi'|N) = \frac{1}{P(N)}\mathrm{Re}\int_0^{\pi}\frac{d\eta_0}{\pi}e^{-i\eta_0 N}n(\xi,\xi'|\eta_0), \quad (84)$$

$$N = \int d\xi\, n(\xi,\xi|N), \quad (85)$$

$$\sum_{k=0}^{2\Omega} n_k = \sum_{N=0}^{2\Omega} NP(N), \quad (86)$$

which as expected has the correct normalization.

As discussed in Ref. [16] the densities (80) and (81) can be used to evaluate the number projected energy of a system as follows

$$E(N) = \frac{1}{P(N)}\mathrm{Re}\int_0^{\pi}\frac{d\eta_0}{\pi}e^{-i\eta_0 N} \quad (87)$$

$$\times\int d\xi\,\mathcal{E}[n(\xi,\xi|\eta_0),...], \quad (88)$$

$$P(N) = \mathrm{Re}\int_0^{\pi}\frac{d\eta}{\pi}e^{-iN\eta_0}\langle|\Phi|\Phi(\eta_0)\rangle, \quad (89)$$

$$\sum_{N=0}^{2\Omega}P(N) = 1, \quad (90)$$

$$\sum_{N=0}^{2\Omega}E(N)P(N) = \int d\xi\,\mathcal{E}[n(\xi,\xi|\eta_0),...]_{\eta_0=0}, \quad (91)$$

and unlike the prescriptions suggested in the past [2–8], these projected densities have no singularities. This aspect was discussed in Ref. [16], and it is also evident from their definitions, as the needed overlaps to evaluate these densities and their derivatives $\langle\Phi|\Phi(\epsilon,\eta_0)\rangle$ have by construction no singularities.

VIII. SIMULTANEOUS PROJECTION ON PARTICLE NUMBER AND A FISSION FRAGMENT INTRINSIC SPIN

One can introduce the transformation of the v-components of the qpwfs when applying a projection operator. The overlap matrix element (for one kind of nucleons) is in this case $\langle\Phi|\Phi(\eta_0,\eta^{\rm F},\beta)\rangle$ is given by

$$\langle\Phi|\Phi(\eta_0,\eta^{\rm F},\beta)\rangle = \sqrt{\det\left[\delta_{kl}+O_{kl}(\eta_0,\eta^{\rm F},\beta^{\rm F})\right]}, \quad (92)$$

$$O_{kl}(\eta_0,\eta^{\rm F},\beta) = \langle {\rm v}_k|e^{2i\eta_0}e^{i\eta^{\rm F}\Theta^{\rm F}}e^{iJ_x^{\rm F}\beta^{\rm F}}-1|{\rm v}_l\rangle, \quad (93)$$

using an obvious generalization of the argumentation presented in Section II. The practical advantage of using this type of angular momentum operator becomes clear when one considers simulations, where nuclei are placed in rectangular boxes. While the v-components of the qpwfs are localized around the center of mass of a fragment and their rotated support remain localized in such a localized spatial domain, the u-components are fully delocalized [29] and their rotated support is ill defined in such simulation boxes.

The intrinsic spin of corresponding fragment is $\boldsymbol{J}^{\rm F} = \int dxdy\,\psi^\dagger(x)\psi(y)\langle x|\boldsymbol{j}^F|y\rangle$ [16], where

$$\langle x|\boldsymbol{j}^F|y\rangle \quad (94)$$
$$= \langle x|\Theta^{\rm F}(\boldsymbol{r})[(\boldsymbol{r}-\boldsymbol{R}^{\rm F})\times(\boldsymbol{p}-m\boldsymbol{v}^{\rm F})+\boldsymbol{s}]\Theta^F(\boldsymbol{r})|y\rangle,$$

and $\boldsymbol{r}$ and $\boldsymbol{p}$ are the nucleon coordinate and momentum, $\boldsymbol{s}$ its spin, m the nucleon mass, $\boldsymbol{R}^{\rm F}$ and $\boldsymbol{v}^{\rm F}$ are the center of mass and the center of mass velocity of the respective FF, and $\Theta^{\rm F}(\boldsymbol{r})=1$ only in a finite volume centered around that FF and otherwise $\Theta^{\rm F}(\boldsymbol{r})\equiv 0$.

The probability that a FF emerges with $N^{\rm F}$ particle number and total intrinsic spin $J^{\rm F}$ in the fission of an axially symmetric even-even nucleus, is given by, see also Refs. [16, 30],

$$P(N,N^{\rm F},J^{\rm F}) = (2J+1)\int_{-\pi/2}^{\pi/2}\frac{d\eta_0}{\pi}\int_{-\pi}^{\pi}\frac{d\eta^{\rm F}}{2\pi}\int_0^\pi d\beta^{\rm F}\sin\beta^{\rm F}$$
$$\times\langle\Phi|\Phi(\eta_0,\eta^{\rm F},\beta^{\rm F})\rangle P_J(\cos\beta^{\rm F}), \quad (95)$$

where $P_J(x)$ is a Legendre polynomial. This formula has a straightforward extension to projecting simultaneously the particle and the intrinsic spins of both FFs using the qpwfs overlap

$$\langle {\rm v}_k|e^{2i\eta_0}e^{i\eta^{\rm F}\Theta^{\rm F}}e^{iJ_x^{\rm L}\beta^{\rm L}}e^{iJ_x^{\rm H}\beta^{\rm H}}-1|{\rm v}_l\rangle, \quad (96)$$

where one can use for F either L or H. These equations are generalizations of those used recently in Ref. [18], where particle projection and double FF intrinsic spins distributions were not considered.

IX. DOUBLE NUMBER PROJECTION FOR AN ONE-BODY OBSERVABLE

Now consider the overlap $\langle\Phi|\Phi(\epsilon,\eta_0,\eta^{\rm F})\rangle$, for the transformation

$${\rm u}_n(\xi,\epsilon,\eta) = {\rm u}_n(\xi),$$
$${\rm v}_n(\xi,\epsilon,\eta_0,\eta^{\rm F}) = [1+2\epsilon\hat{Q}^{\rm F}]e^{2i\eta_0}e^{i\eta^{\rm F}\Theta^{\rm F}}{\rm v}_n(\xi), \quad (97)$$

where

$$\hat{Q}^{\rm F} = \int d\xi d\xi'\langle\xi|\Theta^{\rm F}Q\Theta^{\rm F}|\xi'\rangle\psi^\dagger(\xi)\psi(\xi') \quad (98)$$

and evaluate $q(\eta_0,\eta^{\rm F})$

$$q(\eta_0,\eta^{\rm F}) = \left.\frac{d\langle\Phi|\Phi(\epsilon,\eta_0,\eta_{\rm F})\rangle}{d\epsilon}\right|_{\epsilon=0} \quad (99)$$
$$= \langle\Phi|\Phi(\eta_0,\eta^{\rm F})\rangle e^{2i\eta_0}e^{i\eta^{\rm F}}\sum_{kl}\langle {\rm v}_k|\hat{Q}^{\rm F}|{\rm v}_l\rangle\, a_{lk}(\eta_0,\eta^{\rm F}),$$

$$\delta_{km} = \sum_l[\delta_{kl}+\langle {\rm v}_k|e^{2i\eta_0}e^{i\eta^{\rm F}\Theta^{\rm F}}-1|{\rm v}_l\rangle]\,a_{lm}(\eta_0,\eta^{\rm F}), \quad (100)$$

and thus one can evaluate the particle number projected value of $\hat{Q}^{\rm F}$

$$Q(N,N^{\rm F}) \quad (101)$$
$$= \int_{-\pi/2}^{\pi/2}\frac{d\eta_0}{\pi}\int_{-\pi}^{\pi}\frac{d\eta^{\rm F}}{2\pi}e^{-iN\eta_0-i\eta^{\rm F}N^{\rm F}}q(\eta_0,\eta^{\rm F}).$$

If the overlap $\langle\Phi|\Phi(\eta_0,\eta^{\rm F})\rangle$ vanishes then the inverse matrix $a_{lm}(\eta)$ does not exist. However, the determinant $\det\left[\delta_{kl}+\langle {\rm v}_k|e^{2i\eta_0}e^{i\eta^{\rm F}\Theta^{\rm F}}(1+2\epsilon Q^{\rm F})-1|{\rm v}_l\rangle\right]$ clearly has no singularity for $\epsilon=0$, which implies that all these formulas are well defined everywhere. The formulas for the double projected number and anomalous densities, and the total energy can be derived following the steps outlined in previous sections.

X. CORRELATIONS BETWEEN INTRINSIC SPINS OF THE FISSION FRAGMENTS

A quantity of great interest if the correlation between the magnitudes and the relative orientations of the FF intrinsic spins [31–34]. This correlation can be evaluated by generalizing Eq. (93), using the canonical basis, to the case of two FFs

$$\langle\Phi|\Phi(\eta_0,\eta^{\rm L},\beta^{\rm L},\beta^{\rm H})\rangle \quad (102)$$
$$= \sqrt{\det\left[\delta_{kl}+O_{kl}(\eta_0,\eta^{\rm L},\beta^{\rm L},\beta^{\rm H})\right]},$$
$$O_{kl}(\eta_0,\eta^{\rm L},\beta^{\rm L},\beta^{\rm H}) \quad (103)$$
$$= \langle {\rm v}_k|e^{2i\eta_0}e^{i\eta^{\rm L}\Theta^{\rm L}}e^{i\boldsymbol{J}^{\rm L}\cdot\boldsymbol{n}^{\rm L}\beta^{\rm L}}e^{i\boldsymbol{J}^{\rm H}\cdot\boldsymbol{n}^{\rm H}\beta^{\rm H}}-1|{\rm v}_l\rangle,$$

where $\boldsymbol{n}^{\rm L,H}$ are two independent unit vectors. Since both N and $N^{\rm L}$ are fixed there is no need of a projection on $N^{\rm H}$. One can simplify the projection operator in this matrix element

$$e^{2i\eta_0}e^{i\eta^{\rm L}\Theta^{\rm L}}e^{i\boldsymbol{J}^{\rm L}\cdot\boldsymbol{n}^{\rm L}\beta^{\rm L}}e^{i\boldsymbol{J}^{\rm H}\cdot\boldsymbol{n}^{\rm H}\beta^{\rm H}}-1 \quad (104)$$
$$=(e^{2i\eta_0}-1)$$
$$+e^{2i\eta_0}\Theta^{\rm L}(e^{i\eta^{\rm L}}e^{i\boldsymbol{J}^{\rm L}\cdot\boldsymbol{n}^{\rm L}\beta^{\rm L}}-1)$$
$$+e^{2i\eta_0}\Theta^{\rm H}(e^{i\boldsymbol{J}^{\rm H}\cdot\boldsymbol{n}^{\rm H}\beta^{\rm H}}-1).$$

Even without performing FF particle projections, by ignoring the dependence of this overlap on $\eta^{0,\mathrm{L}}$, one can extract valuable information about the correlations between the relative orientations of the FF intrinsic spins, using the simpler overlap

$$O_{kl}(\beta^{\mathrm{L}},\beta^{\mathrm{H}}) = \langle \mathrm{v}_k| e^{i\boldsymbol{J}^{\mathrm{L}}\cdot\boldsymbol{n}^{\mathrm{L}}\beta^{\mathrm{L}}} e^{i\boldsymbol{J}^{\mathrm{H}}\cdot\boldsymbol{n}^{\mathrm{H}}\beta^{\mathrm{H}}} - 1|\tilde{\mathrm{v}}_l\rangle \tag{105}$$
$$= \langle \tilde{\mathrm{v}}_k|\Theta^{\mathrm{L}}[e^{i\boldsymbol{J}^{\mathrm{L}}\cdot\boldsymbol{n}^{\mathrm{L}}\beta^{\mathrm{L}}}-1]|\mathrm{v}_l\rangle + \langle \mathrm{v}_k|\Theta^{\mathrm{H}}[e^{i\boldsymbol{J}^{\mathrm{H}}\cdot\boldsymbol{n}^{\mathrm{H}}\beta^{\mathrm{H}}}-1]|\mathrm{v}_l\rangle$$

and using a small set of relative angles $\boldsymbol{n}^{\mathrm{L}}\cdot\boldsymbol{n}^{\mathrm{H}} = \cos\beta_{\mathrm{LH}}$. However, no difference was observed between the two cases when $\hat{\boldsymbol{n}}^{\mathrm{L}}\cdot\hat{\boldsymbol{n}}^{\mathrm{H}} = \pm 1$ in the work reported in Ref. [18].

There is no advantage in this case to use the canonical basis and one can proceed exactly as in Ref. [35] and use the original basis $\mathrm{v}_{k,l}(\xi)$ for axially symmetric FFs.

XI. THE ORBITAL ANGULAR MOMENTUM IN SPONTANEOUS FISSION

The spontaneous fission of ^{252}Cf is a particularly important and very clean case to discuss. Since this even-even nucleus has a zero spin in its ground state the FF intrinsic spins and angular momentum satisfy the trivial relation

$$\boldsymbol{J}^{\mathrm{L}} + \boldsymbol{J}^{\mathrm{H}} + \boldsymbol{\Lambda} = 0 \tag{106}$$

and the distribution of the FFs orbital angular momentum can then be extracted. One can project on the sum of the two FF intrinsic spins with

$$P(\Lambda) = \frac{2\Lambda+1}{2}\int_0^\pi d\beta \sin\beta_0\, P_\Lambda(\cos\beta_0)\langle\Phi|\Phi(\beta_0)\rangle, \tag{107}$$
$$\langle\Phi|\Phi(\beta_0)\rangle = \sqrt{\det[\delta_{kl} + O^{\Lambda}_{kl}(\beta_0)]}, \tag{108}$$

where

$$O^{\Lambda}_{kl}(\beta_0) = \sum_{\mathrm{F=L,H}} \langle \mathrm{v}_k|\Theta^{\mathrm{F}}[e^{iJ^{\mathrm{F}}_x\beta_0}-1]|\mathrm{v}_l\rangle. \tag{109}$$

According to Eq. (106) in the case of ^{252}Cf one has $e^{-i\Lambda_x\beta_0} = e^{i(J^{\mathrm{L}}_x+J^{\mathrm{H}}_x)\beta_0}$ and in this case the projection on Λ is equivalent to the projection on the sum of the FF intrinsic spins, if the total wave function has exactly the quantum numbers 0^+, see discussion below too. This type of projector is in fact a projector on the combined FF intrinsic spins. Notice that one can flip the sign of β_0 without any consequence.

One can also add total and fragment particle projections for more detailed information using the following qpwfs overlaps

$$\begin{aligned} O^{\Lambda}_{kl}(\eta_0,\beta_0) &= (e^{2i\eta_0}-1)\langle \mathrm{v}_k|\mathrm{v}_l\rangle \\ &+ e^{2i\eta_0}\langle \mathrm{v}_k|\Theta^{\mathrm{L}}(e^{iJ^{\mathrm{L}}_x\beta_0}-1)|\mathrm{v}_l\rangle \\ &+ e^{2i\eta_0}\langle \mathrm{v}_k|\Theta^{\mathrm{H}}(e^{iJ^{\mathrm{H}}_x\beta_0}-1)|\mathrm{v}_l\rangle, \end{aligned} \tag{110}$$
$$\begin{aligned} O^{\Lambda}_{kl}(\eta_0,\eta^{\mathrm{L}},\beta_0) &= (e^{2i\eta_0}-1)\langle \mathrm{v}_k|\mathrm{v}_l\rangle \\ &+ e^{2i\eta_0}\langle \mathrm{v}_k|\Theta^{\mathrm{L}}(e^{i\eta^{\mathrm{L}}+iJ^{\mathrm{L}}_x\beta_0}-1)|\mathrm{v}_l\rangle \\ &+ e^{2i\eta_0}\langle \mathrm{v}_k|\Theta^{\mathrm{H}}(e^{iJ^{\mathrm{H}}_x\beta_0}-1)|\mathrm{v}_l\rangle. \end{aligned} \tag{111}$$

In the general case Eq. (106) should read

$$\boldsymbol{J}^{\mathrm{L}} + \boldsymbol{J}^{\mathrm{H}} + \boldsymbol{\Lambda} = \boldsymbol{S}_0, \tag{112}$$

where $\boldsymbol{S}_0$ is the initial spin of the fissioning compound nucleus and Eq. (107) will provide the probability distribution $P(|\boldsymbol{\Lambda}-\boldsymbol{S}_0|)$ only.

One can project simultaneously on both intrinsic FF spins and the FFs orbital angular momentum using the overlap

$$\begin{aligned} &O_{kl}(\beta^{\mathrm{L}}+\beta_0,\beta^{\mathrm{H}}+\beta_0) \\ &= \langle \mathrm{v}_k|e^{iJ^{\mathrm{L}}_x\beta^{\mathrm{L}}} e^{iJ^{\mathrm{H}}_x\beta^{\mathrm{H}}} e^{i(J^{\mathrm{L}}_x+J^{\mathrm{H}}_x)\beta_0} - 1|\mathrm{v}_l\rangle \\ &= \sum_{\mathrm{F=L,H}} \langle \mathrm{v}_k|\Theta^{\mathrm{F}}[e^{iJ^{\mathrm{F}}_x(\beta^{\mathrm{F}}+\beta_0)}-1]|\mathrm{v}_l\rangle. \end{aligned} \tag{113}$$

This type of overlap depends only on two angles $\beta^{\mathrm{F}}+\beta_0$, where $\mathrm{F} = \mathrm{L},\mathrm{H}$.

One might consider also an additional projection to enforce the value of total angular momentum $\boldsymbol{S}_0$, with the rotation operator

$$P_0 = e^{i(J^{\mathrm{L}}_x+J^{\mathrm{H}}_x+\Lambda_x)\gamma} \tag{114}$$

where Λ_x rotates the entire system around its center of mass. The result of such a combined rotation is a rotation of each FF around its own center of mass by an angle 2γ due to the action of both Λ_x and J^{F}_x, as well as a displacement of each FF along the y-axis by an amount $D^{\mathrm{F}}\gamma$ for small γ, where $D^{\mathrm{L}} = A^{\mathrm{H}}D/A$ and $D^{\mathrm{H}} = A^{\mathrm{L}}D/A$ and D is the FF separation and $A = A^{\mathrm{L}} + A^{\mathrm{H}}$. Such a combined rotation and displacement of the FFs will make the corresponding overlap $\mathcal{O}^{\Lambda}_{kl}(\beta,\gamma)$ an extremely narrow function of γ at $\gamma = 0$. The net results is that the effective integration interval over γ becomes extremely small, which will lead to a negligible correction to Eq. (107).

XII. NUMERICAL ASPECTS

The extraction of a square root from a complex number leads to two possible roots and numerically the continuity of the overlap $\langle\Psi|\Psi(\eta)\rangle$ as a function of η is not ensured. However, one can use the function `unwrap`, a function common in many computer languages to generate a continuous overlap.

An ambiguity can arise sometimes however if one or more occupation probabilities $n_k \equiv 1/2$, in which case the overlap has a zero, but only for $\eta_0 = \pm\pi/2$, and thus irrelevant, as discussed before [16]

In HFB calculations one can find that very deep levels have occupations probabilities very close to 1, but that does not seem to lead to any numerical issues however in our time-dependent simulations, as all our $\beta_l < 1$ and they always come in pairs.

The potential vanishing of the denominator in Eqs. (80) and (81) is compensated by the vanishing of the overlap $\langle\Phi|\Phi(\eta)\rangle$. In the case of double particle projection the equations are a bit more involved.

As the total and fragment average particle numbers $\langle\Phi|\hat{N}|\Phi\rangle = \sum_k\langle \mathrm{v}_k|\mathrm{v}_k\rangle$ and $\langle\Phi|\hat{N}^{\Theta}|\Phi\rangle = \sum_k\langle \mathrm{v}_k|\Theta|^{\mathrm{F}}|\mathrm{v}_k\rangle$ can be rather easily be evaluated, the particle projection can be performed for particle numbers in relatively small windows around these average values only and at most one or two dozen integration points in each variable should suffice as for small values of $|N - \langle\hat{N}\rangle|$ the integrand has only a few oscillations. The evaluation of fragment particle projected values of other observables (intrinsic spin, deformation, etc.) will proceed in a similar fashion as discussed above in this text.

The great advantage of working in the canonical basis when performing a double projection is that it requires a single diagonalization of the overlap $\langle \mathrm{v}_k|\mathrm{v}_l\rangle$ and a single evaluation of the overlap matrix $\langle\tilde{\mathrm{v}}_k|\Theta^{\mathrm{F}}|\tilde{\mathrm{v}}_l\rangle$. The numerical evaluation of the Eq. (59) and its subsequent integration of the angles $\eta_0, \eta^{\mathrm{F}}$ is relatively inexpensive.

When projecting FF intrinsic spins the overlap matrix element $\langle\Phi|\Phi(\eta_0, \eta^{\mathrm{F}}, \beta^{\mathrm{F}})\rangle$ is numerically significant in a relatively small interval around $\beta^{\mathrm{F}} = 0$ [18] and thus only a small number of integration points are necessary to evaluate Eq. (95) for example. The same situation occurs as well in the case of projecting on both FF intrinsic spins and also on the FFs orbital angular momentum. In particular, the projection on FF intrinsic spins and the FFs orbital angular moment um using the qpwfs overlap (113) can be evaluated fast using the Gauss-Legendre quadrature formulas. Since the none of these Intrinsic spins and FFs orbital angular momentum are larger than $50\hbar$ for each angle one can limit the number of quadrature points to at most $n \approx 50$. That number is even further reduced by the fact that any qpwfs overlap is negligible for angles $\pi/3$ (radians) and then only quadrature points in the interval $\beta_0 + \beta^{\mathrm{F}} \in [0, 0.7]$, a significant reduction of the number of quadrature points.

XIII. CONCLUSIONS

I presented a new set of formulas for restoring broken symmetries in nuclear systems. These formulas are particularly useful when performing static and time-dependent nuclear energy density calculations. A new qualitative element of the present formalism is the absence of singularities for one-body densities, which plagued previous prescriptions, see Section VII. Even though the simultaneous restoring of the broken particle numbers of the total system and of the reaction fragment symmetries require multiple projections, they appear feasible, see recent study [8, 35].

Acknowledgments

The funding from the Office of Science, Grant No. DE-FG02-97ER41014 and also provided in part by NNSA cooperative Agreement DE-NA0003841 is greatly appreciated.

[1] P. Ring and P. Schuck, *The Nuclear Many-Body Problem*, 1st ed. (Springer-Verlag, Berlin Heidelberg New York, 2004).

[2] M. Anguiano, J.L. Egido, and L.M. Robledo, "Particle number projection with effective forces," Nucl. Phys. A **696**, 467 (2001).

[3] L. M. Robledo, "Particle number restoration: its implementation and impact in nucelar structure calculations," Int. J. Mod. Phys. E **16**, 337 (2007).

[4] J. Dobaczewski, M. V. Stoitsov, W. Nazarewicz, and P.-G. Reinhard, "Particle-number projection and the density functional theory," Phys. Rev. C **76**, 054315 (2007).

[5] D. Lacroix, T. Duguet, and M. Bender, "Configuration mixing within the energy density functional formalism: Removing spurious contributions from nondiagonal energy kernels," Phys. Rev. C **79**, 044318 (2009).

[6] M. Bender, T. Duguet, and D. Lacroix, "Particle-number restoration within the energy density functional formalism," Phys. Rev. C **79**, 044319 (2009).

[7] T. Duguet, M. Bender, K. Bennaceur, D. Lacroix, and T. Lesinski, "Particle-number restoration within the energy density functional formalism: Nonviability of terms depending on noninteger powers of the density matrices," Phys. Rev. C **79**, 044320 (2009).

[8] B. Bally and M. Bender, "Projection on particle number and angular momentum: Example of triaxial Bogoliubov quasiparticle states," Phys. Rev. C **103**, 024315 (2021).

[9] D. L. Hill and J. A. Wheeler, "Nuclear Constitution and the Interpretation of Fission Phenomena," Phys. Rev. **89**, 1102 (1953).

[10] J. J. Griffin and J. A. Wheeler, "Collective Motions in Nuclei by the Method of Generator Coordinates," Phys. Rev. **108**, 311 (1957).

[11] K. Goeke and P.-G. Reinhard, "The Generator-Coordinate-Method with conjugate parameters and the unification of microscopic theories for large amplitude collective motion," Ann. Phys. **124**, 249 (1980).

[12] M. Verriere and D. Regnier, "The Time-Dependent Generator Coordinate Method in Nuclear Physics," Frontier in Physics **8**, 233 (2020).

[13] A. Bulgac, "Local-density-functional theory for superfluid fermionic systems: The unitary Fermi gas," Phys. Rev. A **76**, 040502 (2007).

[14] A. Bulgac, "Time-Dependent Density Functional Theory and the Real-Time Dynamics of Fermi Superfluids," Ann. Rev. Nucl. and Part. Sci. **63**, 97 (2013).

[15] A. Bulgac, "Time-Dependent Density Functional Theory for Fermionic Superfluids: from Cold Atomic gases, to Nuclei and Neutron Star Crust," Physica Status Solidi B **256**, 1800592 (2019).

[16] A. Bulgac, "Projection of good quantum numbers for reaction fragments," Phys. Rev. C **100**, 034612 (2019).

[17] A. Bulgac, "The Long Journey from Ab Initio Calculations to Density Functional Theory for Nuclear Large Amplitude Collective Motion," J. Phys. G: Nucl. Part. Phys. **37**, 064006 (2010).

[18] A. Bulgac, I. Abdurrahman, S. Jin, K. Godbey, N. Schunck, and I. Stetcu, "Fission fragment intrinsic spins and their correlations," Phys. Rev. Lett. **126**, 142502 (2021).

[19] A. Bulgac, "The angular correlation between the fission fragment intrinsic spins," (2021), arXiv:2108.07268.

[20] C. Bloch and A. Messiah, "The canonical form of an antisymmetric tensor and its application to the theory of superconductivity," Nucl. Phys. **39**, 95 (1962).

[21] R. Balian and E. Brezin, "Nonunitary Bogoliubov transformations and extension of Wick's theorem," Nuovo Cimento B **64**, 37 (1969).

[22] C. Simenel, "Particle Transfer Reactions with the Time-Dependent Hartree-Fock Theory Using a Particle Number Projection Technique," Phys. Rev. Lett. **105**, 192701 (2010).

[23] N. Onishi and S. Yoshida, "Generator coordinate method applied to nuclei in the transition region," Nucl. Phys. **80**, 367 (1966).

[24] G. Scamps and D. Lacroix, "Effect of pairing on one- and two-nucleon transfer below the coulomb barrier: A time-dependent microscopic description," Phys. Rev. C **87**, 014605 (2013).

[25] M. Verriere, N. Schunck, and D. Regnier, "Microscopic calculation of fission product yields with particle-number projection," Phys. Rev. C **103**, 054602 (2021).

[26] M. Verriere and M. R. Mumpower, "Improvements to the macroscopic-microscopic approach of nuclear fission," Phys. Rev. C **103**, 034617 (2021).

[27] J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Westview Press, Reading, MA, 1998).

[28] R J Furnstahl, "Density functional theory: methods and problems," J. Phys. G: Nucl. Part. Phys. **31**, S1357–S1366 (2005).

[29] A. Bulgac, "Hartree-Fock-Bogoliubov approximnation for finite systems (1980)," arXiv:nucl-th/9907088.

[30] G. F. Bertsch, T. Kawano, and L. M. Robledo, "Angular momentum of fission fragments," Phys. Rev. C **99**, 034603 (2019).

[31] R. Vogt and J. Randrup, "Angular momentum effects in fission," Phys. Rev. C **103**, 014610 (2021).

[32] J. N. Wilson, D. Thisse, M. Lebois, N. Jovancevic, D. Gjestvang, R. Canavan, M. Rudigier, D. Etasse, R-B. Gerst, L. Gaudefroy, E. Adamska, P. Adsley, A. Algora, M. Babo, K. Belvedere, J. Benito, G. Benzoni, A. Blazhev, A. Boso, S. Bottoni, M. Bunce, R. Chakma, N. Cieplicka-Orynczak, S. Courtin, M. L. Cortes, P. Davies, C. Delafosse, M. Fallot, B. Fornal, L. Fraile, A. Gottardo, V. Guadilla, G. Hafner, K. Hauschild, M. Heine, C. Henrich, I. Homm, F. Ibrahim, Ł. W. Iskra, P. Ivanov, S. Jazrawi, A. Korgul, P. Koseoglou, T. Kroll, T. Kurtukian-Nieto, L. Le Meur, S. Leoni, J. Ljungvall, A. Lopez-Martens, R. Lozeva, I. Matea, K. Miernik, J. Nemer, S. Oberstedt, W. Paulsen, M. Piersa, Y. Popovitch, C. Porzio, L. Qi, D. Ralet, P. H. Regan, K. Rezynkina, V. Sanchez-Tembleque, S. Siem, C. Schmitt, P. A. Soderstrom, C. Surder, G. Tocabens, V. Vedia, D. Verney, N. Warr, B. Wasilewska, J. Wiederhold, M. Yavahchova, F. Zeiser, and S. Ziliani, "Angular momentum generation in nuclear fission," Nature **590**, 566 (2021).

[33] P. Marević, N. Schunck, J. Randrup, and R. Vogt, "Angular momentum of fission fragments from microscopic theory," Phys. Rev. C **104**, L021601 (2021).

[34] J. Randrup and R. Vogt, "Generation of Fragment Angular Momentum in Fission," Phys. Rev. Lett. **127**, 062502 (2021).

[35] A. Bulgac, I. Abdurrahman, K. Godbey, and I. Stetcu, "Fragment Intrinsic Spins and Fragments' Relative Orbital Angular Momentum in Nuclear Fission," (2021), arXiv:2108.03763.