Projection of good quantum numbers for reaction fragments

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In reactions, the wave packets of the emerging products typically are not eigenstates of particle number operators or any other conserved quantities, and their properties are entangled. I describe a particle projection technique in parts of space, which eschews the need to evaluate Pfaffians in the case of overlap of generalized Slater determinants or Hartree-Fock-Bogoliubov type of vacua. The extension of these formulas for calculating either angular momentum or particle projected energy distributions of the reaction fragments are presented as well. The generalization to simultaneous particle and angular momentum projection of various reaction fragment observables is straightforward.

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I. INTRODUCTION

In practice, sometimes one is interested in decomposing a many-nucleon wave function restricted to a part of the space into components with an integer number of fermions as typically the fragment wave function is not characterized by a good particle number.

Even if two initial colliding nuclei are characterized by good particle and other good quantum numbers, the emerging reaction fragments are a superposition of nuclei with many possible quantum numbers allowed by conservation laws. When the fragments are so far apart after the collision that any interaction between them is negligible, by performing a measurement of the particle composition of one fragment at once, leads to a well-defined particle number in the other fragment in an obvious generalization of Einstein *et al.* [1] "spooky action at a distance." But unlike in the case of Schrödinger's cat, in this case, there are more than two possible outcomes. The situation becomes even more complex when there are more than two fragments in the final state. Reaction fragments after exchanging particles, energy, angular momenta,..., emerge entangled.

A simple example is that of the collision of a hydrogen atom with a positively charged naked ion. After the collision, when the proton and the ion are infinitely separated, one can find the electron wave function fragmented between the potential well of the initial hydrogen atom and the potential well of the initially naked ion. If one were to make a measurement of where the electron is, one would find it present with different probabilities attached to the proton, to the ion, or even to a free electron. These probabilities are straightforward to evaluate as the integral $\int_{P,I} d\mathbf{r}|\phi(\mathbf{r})|^2$ over either the proton (P) or the ion (I) region of space will give the probabilities to find the electron attached to either the proton or the ion. If these probabilities do not add up to one, that would tell us that the electron has been ejected with some finite probability.

In the case of a many-particle system, the evaluation of the probability to find an integer particle number in either of the emerging nuclear systems is a bit more convoluted, and that will be discussed in this paper with the emphasis on the case of the collision of partners with pairing correlations. The relatively simple example of the collision of "two hydrogen atoms" is discussed in the next section. A more complicated case is that of two nuclei colliding within the Hartree-Fock approximation and that was considered in Ref. [2] and it will be reviewed in the next section. After the collision, the receding wave packets are typically not characterized by good particle numbers. The initial target and projectile nuclei can be described by nonoverlapping Slater determinants. However, after they come into contact, the single-particle wave functions of the initially separated nuclei evolve in the common mean field of the combined nuclear system. Upon separation, the projectile and targetlike nuclei end up with different numbers of nucleons and the single-particle wave functions of the initially separated partners are fragmented with components present in both emerging nuclear systems, and some nucleons might be even knocked out.

In Sec. II, I will review the particle projection in the case of normal nuclei (no pairing correlations), which is the limiting case of the superfluid nuclei when pairing gap vanishes. In Sec. III, I will present the case of superfluid nuclei treated in the Bardeen-Cooper-Schrieffer (BCS) approximation, which is formally equivalent to treating pairing correlation in the canonical basis [3–5]. The projection in the case of generalized Slater determinants is described in Sec. IV. Extensions of the projection method introduced in this paper to angular momentum distributions and particle projected energy are described in a somewhat brief, although full manner, in Secs. V and VI. As this is a relatively short paper, the main conclusions from the abstract, and others sections are not reiterated again at the end.

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II. PROJECTING THE PARTICLE NUMBER IN PART OF THE SPACE IN THE CASE OF A SINGLE SLATER DETERMINANT

I assume that the space has two (or more) partitions, the "left" ($z < 0$) and the "right" ($z > 0$) half-spaces, characterized by the corresponding particle number operators $\hat{N}_{\rm L,R}$,

$$\hat{N}_{\rm L,R} = \int d\xi\, \Theta(\mp z)\psi^\dagger(\xi)\psi(\xi), \tag{1}$$

where $\psi^\dagger(\xi)$ and $\psi(\xi) = \sum_n a_n\phi_n(\xi)$ are field operators, $\phi_n(\xi) = \langle\xi|n\rangle = \langle 0|\psi(\xi)a_n^\dagger|0\rangle$, $|0\rangle$ is the vacuum state, $\xi = \mathbf{r}, \sigma$ stands for spatial $\mathbf{r} = (x, y, z)$, spin $\sigma = \uparrow, \downarrow$, and isospin $\tau = n, p$ coordinates, $\Theta(z)$ is the Heaviside function, and the integral stands for the integral over spatial coordinates and the summation of spin coordinates. $a_n^\dagger$ and a_n are the creation and annihilation operators for single-particle states with wave-functions $\phi_n(\xi)$. The total average numbers of particles in the left and right half-spaces are naturally given by the expressions,

$$N_{\rm L,R} = \int d\xi\, \Theta(\mp z)\sum_{n=1}^{A}|\phi_n(\xi)|^2, \tag{2}$$

where the sum is over occupied single-particle states. In the subsequent formulas, one should make a distinction between the operator $\hat{N}$ and its respective expectation values N. Obviously, one can separate the entire space in arbitrary ways, e.g., the interior and the exterior of a sphere.

The particle projectors on half-space L and R are

$$\hat{P}_{\rm L,R}(N) = \int_{-\pi}^{\pi}\frac{d\eta}{2\pi}e^{i\eta(\hat{N}_{\rm L,R}-N)}, \tag{3}$$

$$e^{i\eta\hat{N}_{\rm L,R}} = 1 + \Theta(\mp z)(e^{i\eta\hat{N}_{\rm L,R}} - 1), \tag{4}$$

$$\langle\phi_n|e^{i\eta\hat{N}_{\rm L,R}}|\phi_m\rangle = \delta_{nm} + (e^{i\eta} - 1)\langle\phi_n|\Theta(z)|\phi_m\rangle. \tag{5}$$

Equation (4) is obtained by expanding the exponential and using $\Theta^2(\mp z) \equiv \Theta(\mp z)$. The probability $P_{\rm R}(N)$ to find exactly N particles in the right half-space is given by [2]

$$P_{\rm R}(N) = \langle\Phi|\hat{P}_{\rm R}(N)|\Phi\rangle = \int_{-\pi}^{\pi}\frac{d\eta}{2\pi}e^{-i\eta N}\langle\Phi|\Phi(\eta)\rangle, \tag{6}$$

where

$$|\Phi\rangle = \prod_{n=1}^{A}a_n^\dagger|0\rangle, \tag{7}$$

$$\langle\Phi|e^{i\eta\hat{N}_R}|\Phi\rangle = \langle\Phi|\Phi(\eta)\rangle = \det[\delta_{mn} + O_{mn}(\eta)], \tag{8}$$

$$O_{nm}(\eta) = (e^{i\eta} - 1)\langle\phi_n|\Theta(z)|\phi_m\rangle. \tag{9}$$

The action of the operator $e^{i\eta\hat{N}_{\rm L,R}}$ on a Slater determinant is equivalent to a fictitious time-dependent evolution of the single-particle states in an external field only $\Theta(\mp z)$ and, therefore,

$$\phi_n(\xi, \eta) = [1 + \Theta(\mp z)(e^{i\eta} - 1)]\phi_n(\xi), \tag{10}$$

where I used the relation $e^{i\eta\Theta(\mp z)} = 1 + \Theta(\mp z)(e^{i\eta} - 1)$.

By diagonalizing at first the matrix $\langle\phi_n|\Theta(z)|\phi_m\rangle$, the numerical calculations are greatly simplified. If the eigenvalues of the overlap matrix $\langle\phi_n|\Theta(z)|\phi_m\rangle$, which is Hermitian positive semidefinite, are $0 \leqslant \alpha_n \leqslant 1$, then

$$P_{\rm R}(N) = \int_{-\pi}^{\pi}\frac{d\eta}{2\pi}e^{-i\eta N}\prod_{n=1}^{A}[1 + (e^{i\eta} - 1)\alpha_n], \tag{11}$$

and similar formulas for the particle number probability $P_{\rm L}(N)$. Note also that $N_{\rm R} = \sum_n \alpha_n$. Obviously, the following relations hold:

$$P_{\rm L}(N) = P_{\rm R}(A - N), \tag{12}$$

$$\sum_{N=0}^{A}P_{\rm L,R}(N) = 1. \tag{13}$$

Note that this formula does not explicitly reveal if nucleons have been knocked out and are not attached to either fragment. It is, however, straightforward to generalize the present formulas to account for emitted nucleons or even clusters.

To illustrate the formalism, let me consider here an idealized case of the collision of two hydrogen atoms, each initially with an electron in its respective ground state when they are infinitely separated ($z \to \infty$ for $t \to -\infty$). The nuclei will follow a classical trajectory, and only the electrons are treated quantum mechanically. The initial electronic wave function is a Slater determinant of two orthonormal single-particle wave functions,

$$\phi_\pm(\mathbf{r}, t) = \tfrac{1}{2}[\phi(\mathbf{r} - \mathbf{z}, t) \pm \phi(\mathbf{r} + \mathbf{z}, t)], \tag{14}$$

$$\int d^3r|\phi(\mathbf{r}, t)|^2 = 1, \tag{15}$$

$$\lim_{t\to-\infty}\int d^3r\,\phi(\mathbf{r} - \mathbf{z}, t)\phi^*(\mathbf{r} + \mathbf{z}, t) = 0, \tag{16}$$

where $\mathbf{z} = (b, 0, z)$ and $2b$ is the impact parameter. After the collision, the Slater determinant will have a similar structure, and the overlap matrix Eq. (9) will be

$$O(\eta) = \frac{e^{i\eta} - 1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \tag{17}$$

which, after using Eq. (11), will lead to exactly one particle per "nucleus" in the final state as one would naturally expect in this case.

III. PROJECTING THE PARTICLE NUMBER IN THE CASE OF GENERALIZED SLATER DETERMINANTS IN THE CANONICAL BASIS

In the case when pairing correlations are present, the nucleus wave function in the canonical basis is given by

$$|\Phi\rangle = \prod_{n=1}^{\Omega}(u_n + v_n a_n^\dagger a_{\bar{n}}^\dagger)|0\rangle, \tag{18}$$

where $u_n^2 + v_n^2 = 1$ and n and $\bar{n}$ denote time-reverse single-particle states. In order to project the particle number, one introduces a rotated in the gauge space wave function, in

which case,

$$u_n \to u_n, \quad v_n \to e^{2i\eta} v_n, \tag{19}$$

$$|\Phi(\eta)\rangle = e^{i\eta\hat{N}}|\Phi\rangle = \prod_{n=1}^{\Omega}(u_n + e^{2i\eta} v_n a_n^\dagger a_{\bar{n}}^\dagger)|0\rangle, \tag{20}$$

$$\Phi_N \propto \int_{-(\pi/2)}^{\pi/2} \frac{d\eta}{\pi} e^{-i\eta N}|\Phi(\eta)\rangle \propto \left(\sum_n \frac{v_n}{u_n} a_n^\dagger a_{\bar{n}}^\dagger\right)^{N/2}, \tag{21}$$

where

$$\hat{N} = \sum_{n=1}^{\Omega}(a_n^\dagger a_n + a_{\bar{n}}^\dagger a_{\bar{n}}), \tag{22}$$

and Φ_N has exactly N particles and

$$|\Phi(\eta)\rangle = \sum_{N=0}^{2\Omega} e^{i\eta N} a_N |\Phi_N\rangle, \tag{23}$$

where $|N\rangle$ have fixed the particle number and only even N particle states contribute to the sum.

In a unitary transformation generated by the operator $e^{i\eta\hat{N}}$, one would consider instead $u_n \to e^{-i\eta} u_n$, $v_n \to e^{i\eta} v_n$, which would lead to a total wave function with a different overall phase $|\tilde{\Phi}(\eta)\rangle = e^{-i\eta\Omega}\prod_{n=1}^{\Omega}(u_n + e^{2i\eta} v_n a_n^\dagger a_{\bar{n}}^\dagger)|0\rangle$. For a zero-range interaction, one should take the limit $\Omega \to \infty$, or, at least, consider $\Omega \gg A$, in which case, $\sum_{n=1}^{\Omega} u_n v_{\bar{n}}^* \to \infty$ for $\Omega \to \infty$ [6] and use the appropriate regularization and renormalization procedures for calculations.

The overlap $\langle\Phi|\Phi(\eta)\rangle = \prod_n(|u_n|^2 + e^{2i\eta}|v_n|^2)$ is a periodic function with period π, and hence, the probability to find exactly N particles (as when N is even and there are $N/2$ pairs) is given by the Fourier transform of $\langle\Phi||\Phi(\eta)\rangle$,

$$P(N) = \int_{-(\pi/2)}^{\pi/2} \frac{d\eta}{\pi} e^{-i\eta N} \prod_{n=1}^{\Omega}[1 + (e^{2i\eta} - 1)|v_n|^2]. \tag{24}$$

Note that the integrand vanishes iff $\eta = \pm\frac{\pi}{2}$ and, at least, for one n also $|v_n|^2 \equiv \frac{1}{2}$, thus, never inside the integration interval.

One can show, by explicit numerical evaluation, that the imaginary part of the quantity $\tilde{Z}(\eta)$,

$$Z(\eta) = \prod_{n=1}^{\Omega}[1 + (e^{2i\eta} - 1)|v_n|^2], \tag{25}$$

$$\tilde{Z}(\eta) = e^{-i\eta N_0} Z(\eta), \tag{26}$$

with $N_0 = \langle\Phi|\hat{N}|\Phi\rangle = 2\sum_{n=1}^{\Omega}|v_n|^2$ is orders of magnitude smaller than its real part if $|v_n|^2$ has a Fermi-like thermal or BCS-like shape and $|v_n|^2 \to 0$ when the upper limit $\Omega \to \infty$, see Fig. 1. $\tilde{Z}(\eta)$ is basically a nonoscillatory function, and $|\tilde{Z}(\eta)| \approx \tilde{Z}(\eta)$ has a bell shape around $\eta = 0$ and may vanish only at $\eta = \pm\frac{\pi}{2}$.

The numerical evaluation of Eq. (24) then becomes much simpler, see Fig. 2, and much more accurate over orders of magnitude as one can instead evaluate

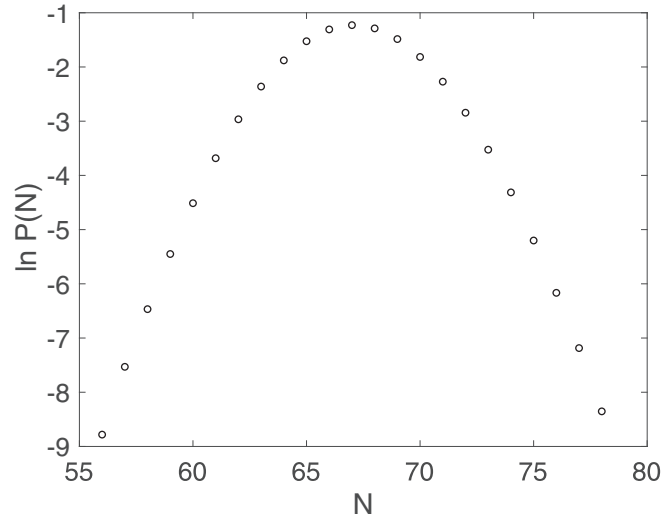

FIG. 1. The probability $P(N)$ of finding N particles in a BCS wave function, derived from the function $Z(\eta)$ in Fig. 2.

$$P(N) = \int_{-(\pi/2)}^{\pi/2} \frac{d\eta}{\pi} e^{-i\eta(N-N_0)} \tilde{Z}(\eta) \tag{27}$$

for a quite large number of values of N around the mean value N_0 using a relatively small number of quadrature points after establishing that the integrand is not a fast oscillating function of η for N very different from N_0. The additional factors $e^{-iN\eta}$ and $e^{iN\eta}$ cancel in Eq. (27) and were introduced only to reveal the properties of the integrand. Since the integral is real, the formula can be simplified

$$P_{\mathrm{R}}(N) = 2\,\mathrm{Re}\int_0^{\pi/2} \frac{d\eta}{\pi} e^{-i\eta N} Z(\eta). \tag{28}$$

IV. PARTICLE PROJECTION IN PART OF THE SPACE IN THE CASE OF A GENERALIZED SLATER DETERMINANT

During time evolution, initially time-reversed single-particle states, in general, cease to satisfy time-reversal symmetry, e.g., in the presence of a time-dependent external magnetic field, and, in that case, one should use the more general formulas below, see Eq. (57). In Eqs. (18), (20), and (24) above, no projection on a half-space is implied.

When discussing time-dependent problems, in particular, well-separated spatially fission fragments, the most convenient representation is in the real space, which I explicitly recapitulate here. The creation and annihilation quasiparticle operators are represented as [5]

$$\alpha_k^\dagger = \int d\xi[u_k(\xi)\psi^\dagger(\xi) + v_k(\xi)\psi(\xi)], \tag{29}$$

$$\alpha_k = \int d\xi[v_k^*(\xi)\psi^\dagger(\xi) + u_k^*(\xi)\psi(\xi)], \tag{30}$$

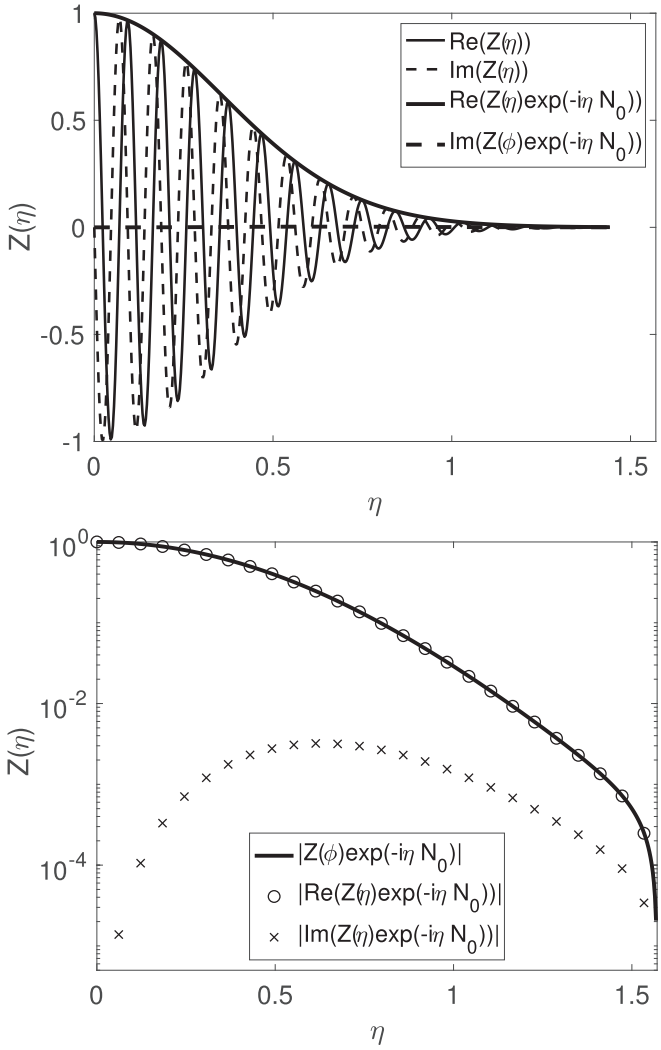

FIG. 2. The function $Z(\eta)$ with the factor $\exp(-i\eta N)$ included or not, evaluated for $|v_n|^2 = \frac{1}{2}[1 - \frac{\varepsilon_n - \mu}{\sqrt{(\varepsilon_n-\mu)^2+\Delta^2}}]$ for a uniform single-particle spectrum $\varepsilon_n \propto n,\ n = 1, 2, \ldots, \infty,\ \mu = 34$, and $\Delta = 2.5$.

and the reverse relations,

$$\psi^\dagger(\xi) = \sum_k [u_k^*(\xi)\alpha_k^\dagger + v_k(\xi)\alpha_k], \tag{31}$$

$$\psi(\xi) = \sum_k [v_k^*(\xi)\alpha_k^\dagger + u_k(\xi)\alpha_k], \tag{32}$$

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

$$\begin{aligned} n(\xi,\xi') &= \langle 0|\psi^\dagger(\xi')\psi(\xi)|0\rangle \\ &= \sum_k v_k^*(\xi)v_k(\xi') = \sum_{l=n,\bar{n}} v_l^2\phi_l^*(\xi)\phi_l(\xi'), \end{aligned} \tag{33}$$

$$\begin{aligned} \kappa(\xi,\xi') &= \langle 0|\psi(\xi')\psi(\xi)|0\rangle \\ &= \sum_k v_k^*(\xi)u_k(\xi') = \sum_{l=n,\bar{n}} u_l v_l \phi_l^*(\xi)\phi_l^*(\xi'), \end{aligned} \tag{34}$$

$$\int d\xi\ \phi_k^*(\xi)\phi_l(\xi) = \delta_{kl}, \tag{35}$$

with $u_l^2 + v_l^2 = 1,\ 0 \leqslant u_l = u_{\bar{l}} \leqslant 1,\ 0 \leqslant v_l = -v_{\bar{l}} \leqslant 1$, and n and $\bar{n}$ denote time-reversed states in the canonical representation [3–5] and where

$$\alpha_k|\Phi\rangle = 0, \quad \langle\Phi|\alpha_k^\dagger = 0, \quad \langle\Phi|\alpha_k\alpha_l^\dagger|\Phi\rangle = \delta_{kl}. \tag{36}$$

In the case of a generalized Slater determinant $|\Phi\rangle$, the total wave function rotated in the gauge space is obtained in a similar manner to the Hartree-Fock case discussed above on projecting on particle number on the right half-space. At this point, I will introduce new kinds of creation and annihilation quasiparticle operators. The result of the gauge rotation on the quasiparticle wave functions, which leads to a similar transformation to Eq. (19), is defined as

$$u_n(\xi,\eta) = u_n(\xi), \quad v_n(\xi,\eta) = e^{2i\eta\Theta(z)}v_n(\xi), \tag{37}$$

which leads to the new types of creation and annihilation operators,

$$\alpha_k^\dagger(\eta) = \int d\xi[u_k(\xi)\psi^\dagger(\xi) + e^{2i\eta\Theta(z)}v_k(\xi)\psi(\xi)], \tag{38}$$

$$\alpha_k(\eta) = \int d\xi[e^{-2i\eta\Theta(z)}v_k^*(\xi)\psi^\dagger(\xi) + u_k^*(\xi)\psi(\xi)]. \tag{39}$$

The anticommutation relations for these operators are

$$\begin{aligned} \{\alpha_k^\dagger(\eta), \alpha_l^\dagger(\eta)\} &= B_{kl} \\ &= \int d\xi[u_k(\xi)v_l(\xi) + v_k(\xi)u_l(\xi)]e^{2i\eta\Theta(z)}, \end{aligned} \tag{40}$$

$$\{\alpha_k^\dagger(\eta), \alpha_l(\eta)\} = \delta_{kl}. \tag{41}$$

These operators are similar to the operators obtained with nonunitary transformations by Balian and Brezin [4], which preserve Eq. (41). By inserting Eqs. (31) and (32) into Eqs. (38) and (39), one can establish that

$$\alpha_k^\dagger(\eta) = \sum_l A_{kl}(\eta)\alpha_l^\dagger + B_{kl}(\eta)\alpha_l, \tag{42}$$

$$\alpha_k(\eta) = \sum_l B_{kl}^*(\eta)\alpha_l^\dagger + A_{kl}^*(\eta)\alpha_l, \tag{43}$$

where these matrices are

$$A_{kl}(\eta) = \int d\xi[u_k(\xi)u_l^*(\xi) + v_k(\xi)v_l^*(\xi)e^{2i\eta\Theta(z)}] \tag{44}$$

$$= \delta_{kl} + (e^{2i\eta} - 1)\int d\xi\ \Theta(z)v_k(\xi)v_l^*(\xi), \tag{45}$$

$$B_{kl}(\eta) = \int d\xi[u_k(\xi)v_l(\xi) + v_k(\xi)u_l(\xi)e^{2i\eta\Theta(z)}] \tag{46}$$

$$= (e^{2i\eta} - 1)\int d\xi\ \Theta(z)v_k(\xi)u_l(\xi) = B_{lk}(\eta). \tag{47}$$

In deriving Eqs. (45) and (47), I took into account that the transformation from field to quasiparticle operators is unitary.

Using the technology described by Balian and Brezin [4], Ring and Schuck [5] in Appendix E, and particularly, the method introduced by Mizusaki *et al.* [7], one can show that

$$|\Phi(\eta)\rangle = \mathcal{N}(\eta)e^{\hat{Z}(\eta)}|\Phi\rangle, \quad \langle\Phi(\eta)|\Phi(\eta)\rangle = 1, \tag{48}$$

where

$$\hat{Z}(\eta) = \sum_{k<l}[A(\eta)^{-1}B(\eta)]^{*}_{kl}\alpha^{\dagger}_{k}\alpha^{\dagger}_{l}, \tag{49}$$

$$\alpha_k(\eta)|\Phi(\eta)\rangle = 0, \quad \langle\Phi|\Phi(\eta)\rangle = \sqrt{\det A} = \mathcal{N}(\eta), \tag{50}$$

with $\mathcal{N}(0) = 1$ and the last relation is known as the Onishi and Yoshida formula [4,5,7,8]. Note that only the antisymmetric part of the matrix $A(\eta)^{-1}B(\eta)$ is contributing in Eq. (49) to the operator $\hat{Z}(\eta)$.

The overlap $\langle\Phi|\Phi(\eta)\rangle$ becomes in this case,

$$\langle\Phi|\Phi(\eta)\rangle = \sqrt{\det\left[\delta_{kl} + (e^{2i\eta} - 1)O_{kl}\right]}, \tag{51}$$

$$O_{kl} = \langle v_l|\Theta(z)|v_k\rangle, \tag{52}$$

and where $v_{k,l}$'s are the v components of the quasiparticle wave functions and the indices k and l run over all single-particle states, e.g., both n and its counterpart $\bar{n}$, for which $u_n = u_{\bar{n}}$ and $v_n = -v_{\bar{n}}$ in the representation where the number density $n(\xi,\xi')$ is diagonal and the anomalous density $\kappa(\xi,\xi')$ is antisymmetric 2×2 block diagonal [3,5]. For stationary states, there is no sign ambiguity in choosing the sign of the square root in Eq. (51) [9]. Again, since the matrix O is Hermitian (and positive semidefinite), it can be diagonalized.

The probability to find N particles in the right half-space is given in this case by

$$P_{\mathrm{R}}(N) = \int_{-(\pi/2)}^{\pi/2}\frac{d\eta}{\pi}e^{-i\eta N}\sqrt{\prod_{l=1}^{2\Omega}[1 + (e^{2i\eta} - 1)\beta_l]}. \tag{53}$$

where $0 \leqslant \beta_l \leqslant 1$ are the eigenvalues of overlap matrix O, see Eq. (52), and

$$\langle\Phi|\Phi(\eta)\rangle = \sqrt{\prod_{l=1}^{2\Omega}[1 + (e^{2i\eta} - 1)\beta_l]}. \tag{54}$$

A factor $[1 + (e^{2i\eta} - 1)\beta_l]$ is zero if and only if both $\eta \equiv \pm\frac{\pi}{2}$ and $\beta_l \equiv \frac{1}{2}$, thus, exactly at the upper and lower limits of the integration interval only. Therefore, there is no ambiguity in this case as well for choosing the sign of the square root.

The above formulas can be simplified a little bit further as $P_{\mathrm{R}}(N)$ is real and Eq. (53) can be reduced to

$$P_{\mathrm{R}}(N) = 2\,\mathrm{Re}\int_{0}^{\pi/2}\frac{d\eta}{\pi}e^{-i\eta N}\sqrt{\prod_{l=1}^{2\Omega}[1 + (e^{2i\eta} - 1)\beta_l]}. \tag{55}$$

With the replacement $\Theta(z) \to 1$ and after the diagonalization of the matrix $\langle v_l|v_k\rangle$, one recovers the canonical basis result, see Eq. (24). The particular case when the generalized Slater determinant $|\Phi\rangle$ is represented in the canonical basis, and when the states n and $\bar{n}$ do not anymore satisfy the time-reversal symmetry, follows from Eq. (53). The comments made above, see Eqs. (26) and (27), about the oscillatory character of the integrand apply here as well. In particular, one also has $N_{\mathrm{R}} = \sum_{l=1}^{2\Omega}\beta_l$. And finally, for the left half-space, one obviously has $P_{\mathrm{L}}(N) = P_{\mathrm{R}}(A - N)$.

Note the difference among Eqs. (9) and (24) (where there is no square root) and Eqs. (51), (53), and (55) (where there is a square root). When pairing correlations vanish, one naively expects that Eqs. (9) and (24) and (51) and (53) should agree. However, in the case of ordinary Slater determinants, the projected value of N and the dimension of the matrix O can be even or odd, and for that reason the integration interval on η is $[-\pi,\pi]$. For generalized Slater determinants, the dimension of matrix O is always even, and the integration interval is now $[-\pi/2,\pi/2]$. When there are degenerate time-reversal orbitals n and $\bar{n}$, after extracting the square root in Eq. (53), one is left with half the number of factors in the product as in the case of Eq. (24) where there is no square root. In Eq. (24), the product runs only over n states but not over their time-reversed partners $\bar{n}$. Therefore, Eq. (24) agrees with Eq. (53) in the case when there are degenerate time-reversed orbitals. One can project in this case only on even particle numbers N in the right half-space. The generalization to a system with pairing correlations and total odd particle numbers is straightforward [5].

Recently Mizusaki *et al.* [7] clarified the reasons why the Onishi and Yoshida formula does not have a sign ambiguity, particularly, in the case when the size of the Fock space is finite as is the case in the overwhelming majority of numerical implementations. They have proven that Onishi and Yoshida [8] and Robledo [10] formulas for the norm overlaps are identical in this case. A different approach to evaluate number of particles in fission fragments was recently suggested by Verriere *et al.* [11].

There is a generalization of Eq. (53) to the case when, in the right half-space, there are fragments with an odd particle number, which can happen, for example, when, during time-dependent evolution, Cooper pairs break up and partners in initially time-reversed orbitals can end up in different half-spaces. This is achieved by replacing $2\eta \to \eta$ in Eq. (37), which leads to obvious changes in the ensuing equations for both even- and odd-N values and the integration interval changes to $[-\pi,\pi]$. Namely,

$$\langle\Phi|\Phi(\eta)\rangle = \sqrt{\det\left[\delta_{kl} + (e^{i\eta} - 1)O_{kl}\right]}, \tag{56}$$

$$P_{\mathrm{R}}(N) = \mathrm{Re}\int_{0}^{\pi}\frac{d\eta}{\pi}e^{-iN\eta}\sqrt{\prod_{l}[1 + (e^{i\eta} - 1)\beta_l]}, \tag{57}$$

where, as before, $0 \leqslant \beta_l \leqslant 1$ are the eigenvalues of matrix O, which was defined in Eq. (52), but now N can be both an even or an odd integer. One can convince oneself that there is no sign ambiguity in extracting the square root in this case either, following the same kind of argument I presented above.

V. EXTENSION TO PROJECTING THE ANGULAR MOMENTUM

In the case of three-dimensional rotations, one can develop a similar projection technique. For simplicity, let me consider a one-parameter group transformation, e.g., rotation around a

single axis $\hat{R}(\eta) = e^{i\hat{J}_x\eta}$ perpendicular to the symmetry axis of a nucleus [12] and the corresponding transformation of the components of the quasiparticle wave functions,

$$u_n(\xi,\eta) \equiv u_n(\xi), \quad v_n(\xi,\eta) = \hat{R}(\eta)v_n(\xi). \tag{58}$$

Typically, one would rotate both u and v components of the quasiparticle wave functions. Since one typically is interested only in the matter densities, it is not necessary to rotate the u components as well, similar to Eqs. (38) and (39). In this case, the overlap matrix element $\langle\Phi|\Phi(\eta)\rangle$ is given by

$$\langle\Phi|\Phi(\eta)\rangle = \sqrt{\det\left[\delta_{kl} + \langle v_l|\hat{R}(\eta)|v_k\rangle - \langle v_l|v_k\rangle\right]}. \tag{59}$$

In the canonical basis, matrix $\langle v_l|v_k\rangle$ is diagonal and since $\hat{R}(\eta) = e^{i\hat{J}_x\eta}$, one can then prove that both matrices $\langle v_l|v_k\rangle$ and $\langle v_l|\hat{R}(\eta)|v_k\rangle$ can be diagonalized simultaneously. Let me denote the eigenvalues of the matrices $\langle v_l|v_k\rangle$ and $\langle v_l|\hat{R}(\eta)|v_k\rangle$ with v_n^2 and $w_n^2 e^{i\lambda_n}$, respectively. The sign of the overlap matrix element $\langle\Phi|\Phi(\eta)\rangle$ is ill defined for some values of η if and only if for, at least, for one n one has $w_n^2 + v_n^2 \equiv 1$ and at the same time inside the integration interval $\lambda \equiv -\pi$. For example, in the case of a nuclei invariant with respect to reflection symmetry $z \to -z$, a rotation by $\eta = \pm\pi$ leads to an identical state and in this case $w_n^2 = v_n^2$ (although not necessarily to $w_n^2 + v_n^2 \equiv 1$). However, the integration interval for η is $[-\pi,\pi]$, and the overlap matrix element vanishes exactly at the limits of the integration integral over η iff $w_n^2 + v_n^2 \equiv 1$, and no ambiguity over the sign of the overlap matrix element $\langle\Phi|\Phi(\eta)\rangle$ arises in this case. The complex valued overlap $\langle\Phi|\Phi(\eta)\rangle$ is expected to be a continuous function of η, and sign ambiguities can arise only if this overlap vanishes strictly inside the interval $(-\pi,\pi)$. In the case of reflection symmetry $z \to -z$, it is sufficient to consider rotations only in the interval $[-\pi/2,\pi/2]$. In addition, axial symmetry in the presence of reflection symmetry $z \to -z$ also implies that one can reduce the integration interval even further to $[0,\pi/2]$.

In the case of the axially symmetric reaction fragments, the individual probabilities can be evaluated using [12]

$$|\Phi\rangle = \sum_J a_J|J0\rangle, \tag{60}$$

$$|a_J|^2 = (2J+1)\int_0^\pi d\eta\, \sin(\eta)\langle\Phi|\Phi(\eta)\rangle P_J(\cos\,\eta), \tag{61}$$

where $|J0\rangle$ is the wave function with total angular momentum J and $J_z = 0$ and P_J is a Legendre polynomial.

VI. EXTENSION TO PROJECTING THE PARTICLE NUMBER FOR OTHER OBSERVABLES

One can define generalized density matrices,

$$n(\xi,\xi'|\eta) = \langle\Phi|\psi^\dagger(\xi')\psi(\xi)|\Phi(\eta)\rangle, \tag{62}$$

$$\kappa(\xi,\xi'|\eta) = \langle\Phi|\psi(\xi')\psi(\xi)|\Phi(\eta)\rangle, \tag{63}$$

$$n_2(\xi_1,\xi_2,\zeta_1,\zeta_2|\eta) = \langle\Phi|\psi^\dagger(\xi_1)\psi^\dagger(\xi_2)\psi(\zeta_2)\psi(\zeta_1)|\Phi(\eta)\rangle, \tag{64}$$

with $\Phi(\eta)\rangle$ defined in Eq. (48). These generalized density matrices are well defined and have no divergencies. Using the Cauchy-Schwarz inequality, it follows immediately that

$$|n(\xi,\xi|\eta)|^2 \leqslant \langle\Phi|\psi^\dagger(\xi)\psi(\xi)|\Phi\rangle\langle\Phi(\eta)|\psi^\dagger(\xi)\psi(\xi)|\Phi(\eta)\rangle,$$

and similar relations for $\kappa(\xi,\xi'|\eta)$ and $n_2(\xi_1,\xi_2,\xi_1,\xi_2|\eta)$. General rules for evaluating such densities have been derived many times, see, e.g., Refs. [4,5,10,13–16]. Alternatively, one can invert Eqs. (38) and (39) to express $\psi^\dagger(\xi)$ and $\psi(\xi)$ in terms of $\alpha_k^\dagger(\eta)$ and $\alpha_k(\eta)$ and, subsequently, use $\langle\Phi|\alpha_k^\dagger = 0$ and $\alpha_k(\eta)|\Phi(\eta\rangle = 0$.

In the case of a density-functional theory (DFT) approach, the total energy of a system is a function(al) of various densities $\mathcal{E}[n(\xi,\xi),\ldots]$, where the ellipses stand for other densities not explicitly shown. The number projected energy in this case is defined as

$$E(N) = \frac{1}{P(N)}\mathrm{Re}\int_0^\pi \frac{d\eta}{\pi} e^{-i\eta N}\mathcal{E}[n(\xi,\xi|\eta),\ldots], \tag{65}$$

in which one has to use the generalized densities in the expression for the energy-density functional. Mathematically, this follows from the definition of a conditional probability and one has

$$\begin{aligned} E(N) &= \frac{\int_0^{2\pi} d\eta\, e^{-iN\eta}\langle\Phi|\hat{H}|\Phi(\eta)\rangle}{\int_0^{2\pi} d\eta\, e^{-iN\eta}\langle\Phi|\Phi(\eta)\rangle} = E_N, \\ \langle\Phi|\hat{H}|\Phi(\eta)\rangle &= \sum_N E_N e^{i\eta N}|a_N|^2, \\ \langle\Phi|\Phi(\eta)\rangle &= \sum_N e^{i\eta N}|a_N|^2, \quad |\Phi\rangle = \sum_N a_N|N\rangle, \end{aligned} \tag{66}$$

if $[\hat{H},\hat{N}] = 0$. In the sums, degeneracies are implied, and $|N\rangle$ are states with fixed particle number N and average energy $E_N = \langle N|\hat{H}|N\rangle$. $E(N)$ can be evaluated with such a formula only if $a_N \neq 0$, thus, iff the trial state $|\Phi\rangle$ has a nonvanishing overlap with state $|N\rangle$. There is an immediate implication in these formulas that within a DFT approach $\mathcal{E}[n(\xi,\xi|\eta),\ldots]$ should be a faithful representation of $\langle\Phi|\hat{H}|\Phi(\eta)\rangle$.

In a similar manner, one can evaluate any other number projected observables or even combine particle and angular momentum projections for reaction fragments. In all the formulas, the $\Theta(z)v_n(\xi)$ components of the quasiparticle wave functions control the projected values of the observables, and thus, all matrix elements extend only over the matter distribution of the reaction fragments in a well-defined spatial region, once the reaction fragments are well separated. Since the overlap between well-separated fragments is vanishingly small, the formal noncommutativity between $\Theta(Z)$ and the angular momentum of a fragment J_x with respect to its own center of mass is irrelevant.

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[1] A. Einstein, B. Podolsky, and N. Rosen, Can quantum-mechanical description of physical reality be considered complete? Phys. Rev. **47**, 777 (1935).
[2] C. Simenel, Particle Transfer Reactions with the Time-Dependent Hartree-Fock Theory Using a Particle Number Projection Technique, Phys. Rev. Lett. **105**, 192701 (2010).
[3] 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).
[4] R. Balian and E. Brezin, Nonunitary Bogoliubov transformations and extension of Wick's theorem, Nuovo Cimento B **64**, 37 (1969).
[5] P. Ring and P. Schuck, *The Nuclear Many-Body Problem*, 1st ed., Theoretical and Mathematical Physics Series No. 17 (Springer-Verlag, Berlin/Heidelberg/New York, 2004).
[6] A. Bulgac and Y. Yu, Renormalization of the Hartree-Fock-Bogoliubov Equations in the Case of a Zero Range Pairing Interaction, Phys. Rev. Lett. **88**, 042504 (2002).
[7] T. Mizusaki, M. Oi, and N. Shimizu, Why does the sign problem occur in evaluating the overlap of HFB wave functions? Phys. Lett. B **779**, 237 (2018).
[8] N. Onishi and S. Yoshida, Generator coordinate method applied to nuclei in the transition region, Nucl. Phys. **80**, 367 (1966).
[9] J. A. Sheikh and P. Ring, Symmetry-projected Hartree–Fock–Bogoliubov equations, Nucl. Phys. A **665**, 71 (2000).
[10] L. M. Robledo, Sign of the overlap of Hartree-Fock-Bogoliubov wave functions, Phys. Rev. C **79**, 021302(R) (2009).
[11] M. Verriere, N. Schunck, and T. Kawano, Number of particles in fission fragments, Phys. Rev. C **100**, 024612 (2019).
[12] G. F. Bertsch, T. Kawano, and L. M. Robledo, Angular momentum of fission fragments, Phys. Rev. C **99**, 034603 (2019).
[13] Q.-L. Hu, Z.-C. Gao, and Y. S. Chen, Matrix elements of one-body and two-body operators between arbitrary HFB multi-quasiparticle states, Phys. Lett. B **734**, 162 (2014).
[14] B. Avez and M. Bender, Evaluation of overlaps between arbitrary fermionic quasiparticle vacua, Phys. Rev. C **85**, 034325 (2012).
[15] T. Mizusaki, M. Oi, F.-Q. Chen, and Y. Sun, Grassmann integral and Balian–Brézin decomposition in Hartree–Fock–Bogoliubov matrix elements, Phys. Lett. B **725**, 175 (2013).
[16] G. F. Bertsch and L. M. Robledo, Symmetry Restoration in Hartree-Fock-Bogoliubov Based Theories, Phys. Rev. Lett. **108**, 042505 (2012).