Framework for Polarized Superfluid Fermion Systems

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I discuss the advantages and disadvantages of several procedures, some known and some new, for constructing stationary states for a system with pairing correlations and an odd number of fermions, using the two chemical potentials framework. One procedure in particular appears to have significant advantages over previously suggested in the literature computational frameworks. Moreover, this framework is applicable to study strongly polarized superfluid nuclei with arbitrarily large polarizations, even or odd, in the presence of very strong external fields.

I. INTRODUCTION

In a time-dependent framework, a major difficulty in studying the dynamics of a superfluid nucleus with an odd number of either protons or/and neutrons is the construction of the initial stationary state. Using the blocking approximation for the initial state could be problematic in the case of time-dependent phenomena. Within the blocking approximation the odd fermion is often described by a single-particle wave function and not by a Bogoliubov quasiparticle wave function, and thus the orthogonality between the two types of fermion wave function cannot be enforced during the time evolution, except within the BCS approximation. Experiments show that the fission of odd or odd-odd nuclei is hindered significantly when compared with the fission of the neighboring even-even nuclei. The unpaired fermion(s) can be found in a state with a relatively high total angular momentum projection on the reaction axis and in that case the presence of an odd fermion can have a strong hindering effect [1–3].

One theoretically method used to describe (static) pairing correlations in a system with an odd number of fermions requires the use of two different chemical potentials for the approximately time-reversed single-particle states. The presence of an odd fermion can lead to a relatively weak time-reversal mean field symmetry breaking and to different mean fields for the partners of the Cooper pair, induced by the polarization effects due to the odd fermion. The two chemical potential approach has been used in Refs. [4–11]. See also the online appendix to Ref. [4] and the actual code used in those calculations [12]. The two chemical potential approach discussed by Bertsch et al. [8] can be implemented only when the quasiparticle states of the closest even (or even-even) system are doubly degenerate. The general approach to describe odd fermion systems used in nuclear physics [13–16], including the two chemical potential framework discussed by Bertsch et al. [8], has the major disadvantage that one needs to know a priori the quantum numbers of the odd fermion. Robledo and Bertsch [17] however have shown that a gradient technique approach [15] is apparently free of this difficulty. Sometimes the implementation of the general approach is construed as gain, as one can determine at once an slew of low lying excited states of the odd or of the odd-odd nucleus, even though the computational price is high. While adding a single extra fermion to an even fermion system can appear as a small perturbation $O(1/A)$, since the low energy spectrum of odd and odd-odd nuclei is relatively dense, a small perturbation can in principle lead to significant change of the nuclear mean field. The question I raise here is: “Can one devise a more transparent and computationally faster framework to describe pairing correlations in odd and odd-odd nuclei?” Since unpolarized fermion systems, or even-even nuclei treat the “spin-up” and “spin-down” fermions identically, naturally there is the need for only one chemical potential. It seems then that since in polarized or odd fermion systems, or in odd and odd-odd nuclei, “spin-ups” and “spin-down” are clearly experience different mean fields, the introduction of two chemical potentials does not need a justification and it seems like the most natural approach.

In Section II I review the Bogoliubov transformation and the definition of various densities for even and odd fermion numbers. In Section III I review a previously suggested framework for odd fermion systems with axial and parity symmetry [8], I introduce a couple of generalizations applicable when and octupole deformation is present, and I discuss their advantages and disadvantages. In Section IV I review the framework designed for the cold atom systems, which has some peculiarities when spin-orbit is absent. In Section V I introduce the optimal two chemical potential framework, which appears to be free of any of the disadvantages of those previously suggested in the literature frameworks for nuclear systems. In the last Section VI I discuss several aspects concerning the optimal numerical implementation of this framework.

II. FORMULATION OF BOGOLIUBOV TRANSFORMATIONS FOR EVEN AND ODD FERMION NUMBERS

First I review the case of a system with an even number of fermions, such as even-even nuclei. The creation
and annihilation quasiparticle operators are represented as [15]

\[ \alpha_k^\dagger = \int d\xi \left[ u_k(\xi)\psi^\dagger(\xi) + v_k(\xi)\psi(\xi) \right], \]
\[ \alpha_k = \int d\xi \left[ v_k^*(\xi)\psi^\dagger(\xi) + u_k^*(\xi)\psi(\xi) \right], \]

and the reverse relations are

\[ \psi^\dagger(\xi) = \sum_k \left[ u_k^*(\xi)\alpha_k^\dagger + v_k(\xi)\alpha_k \right], \]
\[ \psi(\xi) = \sum_k \left[ v_k^*(\xi)\alpha_k^\dagger + u_k(\xi)\alpha_k \right], \]

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

\[ n(\xi, \xi') = \langle \Phi | \psi^\dagger(\xi')\psi(\xi) |\Phi \rangle = \sum_{l=n,\bar{n}} v_{l'}^*(\xi)v_{l}(\xi') = \sum_{l=n,\bar{n}} v_{l'}^*(\xi)\phi^*_l(\xi') \]
\[ \kappa(\xi, \xi') = \langle \Phi | \psi(\xi')\psi^\dagger(\xi) |\Phi \rangle = \sum_{l=n,\bar{n}} v_{l'}^*(\xi)u_{l}(\xi') = \sum_{l=n,\bar{n}} u_{l}v_{l'}(\xi)\phi_l(\xi'), \]

\[ \int d\xi \phi_{l'}^*(\xi)\phi_l(\xi) = \delta_{kl}, \]

with \( u_{l}^2 + v_{l}^2 = 1, 0 \leq u_{l} = u_{\bar{l}} \leq 1, 0 \leq v_{l} = -v_{\bar{l}} \leq 1 \), and \( n \) and \( \bar{n} \) label the time-reversed states \( \phi_l(\xi), \phi^*_l(\xi) \) in the canonical representation [15, 18], and where

\[ \alpha_k |\Phi \rangle = 0, \quad \langle \Phi | \alpha_k^\dagger = 0, \quad \langle \Phi | \alpha_k \alpha_k^\dagger |\Phi \rangle = \delta_{kl}. \]

There is in general no rule on how to separate the quasiparticle operators \( \alpha_k^\dagger, \alpha_k \) into creation and annihilation ones, and one can rename interchange any number of them, and declare the a number of creation operators annihilation operators and vice versa. This is unlike the field operators \( \psi^\dagger(\xi), \psi(\xi) \), which are defined with respect to the true vacuum, \( |\psi(\xi)| \rangle \equiv 0 \). Only by requiring that the quasiparticle vacuum \( |\Phi \rangle \) corresponds to the lowest, or often to a local minimum, of the total energy of an average even number of fermions, one can clearly distinguish between creation and annihilation quasiparticle operators.

In the case of an odd number of fermions the ground state is defined as \( \alpha_{\mu}^\dagger |\Phi \rangle \), where \( \mu \) is an appropriately chosen a priori quasiparticle state, and thus

\[ \alpha_{\mu}|\Phi \rangle = 0, \quad \langle \Phi | \alpha_{\mu}^\dagger = 0, \quad \langle \Phi | \alpha_{\mu} \alpha_{\mu}^\dagger |\Phi \rangle = \delta_{\mu\mu}. \]

Since by definition \( |\Phi \rangle \) corresponds to an average even number of fermions \( N \), the state \( \alpha_{\mu}^\dagger |\Phi \rangle \) should describe an odd number of fermions \( N \pm 1 \), and their corresponding particle parity is given by \((-1)^N = +1 \) or \((-1)^{N \pm 1} = -1\) respectively. Note however, than the state \( \alpha_{\mu}^\dagger |\Phi \rangle \) defined by Eq. (10) does not automatically has an integer average odd number of fermions, as the chemical potential, and therefore the quasiparticle wavefunctions should be correspondingly adjusted. Since

\[ |\Phi \rangle \propto \prod_k \alpha_k |0\rangle, \]

(assuming that \( \alpha_k |0\rangle \neq 0 \) for any \( k \), otherwise see Ring and Schuck [15]) \(^1\) the ground state of an odd fermion system is therefore defined as

\[ \alpha_{\mu}^\dagger |\Phi \rangle \propto \prod_k \alpha_k |0\rangle, \]

where \( |0\rangle \) is the particle vacuum, and thus \( \langle \psi(\xi)|0\rangle \equiv 0 \). The normal number and anomalous densities are in this case

\[ n_{\mu}(\xi, \xi') = \langle \Phi | \alpha_{\mu}\psi^\dagger(\xi')\psi(\xi) |\Phi \rangle = \sum_{k \neq \mu} v_{k}(\xi)v_{k}(\xi') + u_{\mu}(\xi)u_{\mu}(\xi'), \]
\[ \kappa_{\mu}(\xi, \xi') = \langle \Phi | \alpha_{\mu}\psi(\xi')\psi^\dagger(\xi) |\Phi \rangle = \sum_{k \neq \mu} v_{k}(\xi)u_{k}(\xi') + u_{\mu}(\xi)v_{\mu}(\xi'). \]

Thus the major difference from Eqs. (5-6) is the absence of the contribution of the chosen quasiparticle state \( \mu \) in the sum, which is replaced by the “flipped” quasiparticle wavefunction \( (u_{\mu}(x), v_{\mu}(x)) \rightarrow (v_{\mu}^*(x), u_{\mu}^*(x)) \). This quasiparticle state \( \mu \) is chosen so as to minimize the total energy of the system with a fixed odd fermion number. In the case of an odd-odd nucleus one has to naturally chose two such quasiparticle states, one for the neutron and the other for the proton subsystems respectively.

### III. SELF-CONSISTENT EQUATIONS FOR SYSTEMS WITH AN ODD NUMBER OF FERMIONS

Here I describe the two chemical potential framework for a polarized (odd) fermion system. I introduce a new quantum number \( \eta \), the sign of the expectation value of the single-particle angular momentum operator along the axial symmetry axis \( Oz \) and the corresponding operator

\[ S_z = \text{sign}(\hat{J}_z) = \text{sign} \left( \hat{\ell}_z + \frac{\hbar}{2}\sigma_z \right). \]

---

\(^1\) In the case of a finite dimensional Hilbert space it could be problematic to establish if mathematically \( \alpha_{\mu} |\Phi \rangle \neq 0 \), since when \( \int d\xi |\psi_k(\xi)\|^2 \) is smaller then the machine precision the corresponding annihilation operators do not anti-commute anymore and the ordering of the terms in product Eq. (10) can lead to results differing by more than just by a phase.
If $Oz$ is the axial symmetry axis then the quasiparticle wavefunctions are eigenfunctions of $S_z$ with eigenvalues

$$\eta = \text{sign}(m) = \pm 1.$$  \hfill (15)

The self consistent equations are:

$$\begin{pmatrix}
H_{\eta\uparrow\uparrow} & H_{\eta\uparrow\downarrow} \\
H_{\eta\downarrow\uparrow} & H_{\eta\downarrow\downarrow}
\end{pmatrix}
\begin{pmatrix}
u_{k,m,\uparrow} \\
v_{k,m,\downarrow}
\end{pmatrix}
= \begin{pmatrix}
\delta & \Delta \\
-\Delta & 0
\end{pmatrix}
\begin{pmatrix}
u_{k,m,\uparrow} \\
v_{k,m,\downarrow}
\end{pmatrix}, \hfill (16)

H_{\eta\sigma,\sigma} = H_{\sigma\sigma} - \mu - \mu_\eta S_z - Q \quad \text{with} \quad \sigma = \uparrow, \downarrow, \hfill (17)

and where I suppressed the arguments $(r, \sigma)$ for spatial and spin coordinates (isospin is not explicitly displayed). $Q = \sum_l \lambda_l Q_{l0}$ stands for all other necessary constraints, including the corresponding Lagrange multipliers, and $k$ stands for the rest of quantum numbers characterizing the quasiparticle states, apart from $m$. I have also used a short hand notation for the components of the quasiparticle wavefunctions $u_{k,m,\sigma} = u_{k,m}(r, \sigma)$, $v_{k,m,\sigma} = v_{k,m}(r, \sigma)$, where $\sigma = \uparrow, \downarrow$. In this case there are two chemical potentials $\mu - \mu_\eta \pm \mu_\eta$.

The normal partial and total number (and other relevant) densities and also anomalous densities are

$$n_\eta(r, \sigma, \sigma') = \sum_{E_{k,m} > 0} u_{k,m}^*(r, \sigma', \sigma) v_{k,m}(r, \sigma) \delta_{\eta, \text{sign}(m)}, \hfill (18)

n(r, \sigma, \sigma') = n_+(r, \sigma, \sigma') + n_-(r, \sigma, \sigma'), \hfill (19)

\nu(r) = \sum_{E_{k,m} > 0} v_{k,m}^*(r, \downarrow) u_{k,m}(r, \uparrow). \hfill (20)

The Hamiltonian $H(r, \sigma)$ and the pairing potential $\Delta(r, \sigma)$ are functional derivatives of the energy density functional $\mathcal{E}(n, \nu, \tau, \ldots)$

$$H(r, \sigma, \sigma') = \frac{\delta \mathcal{E}(n, \nu, \tau, \ldots)}{\delta n(r, \sigma, \sigma')}, \hfill (21)

\Delta(r) = \frac{\delta \mathcal{E}(n, \nu, \tau, \ldots)}{\delta \nu(r, \uparrow, \downarrow)}. \hfill (22)

The energy density functional of nuclear systems typically depends on the sum $n(r, \sigma, \sigma') = n_+(r, \sigma, \sigma') + n_-(r, \sigma, \sigma')$ alone, while in the case of cold atoms the energy density functional depends on both $n_+(r, \sigma, \sigma')$ separately, as fermions of various flavors can reside in different external potentials. The two chemical potentials $\mu \pm \mu_\eta$ are determined from the condition that the total and partial particle numbers are

$$N = N_+ + N_-, \quad |N_+ - N_-| = 1, \hfill (23)

N_\pm = \int d^3r \sum_{\sigma = \uparrow, \downarrow} n_\pm(r, \sigma, \sigma). \hfill (24)

Notice that the equations for the quasiparticle states with $m > 0$ ($\eta = +1$) and $m < 0$ ($\eta = -1$) respectively have two different chemical potentials $\mu \pm \mu_\eta$, and in both cases the eigenvalues $E_{k,m}$ come also in pairs $(E_{k,m}, -E_{k,m})$, see also Section IV.

The operator $S_z$ can be used in the case of axial symmetry for a nucleus with octupole deformation, unlike the hermitian signature operator $i \exp(-i\tau_j x)$ with eigenvalues $\pm 1$ suggested in Ref. [8]. One can relatively easily use instead of the operator $i \exp(-i\tau_j x)$ the so called simplex operator $i \exp(-i\tau_j x) P$ [14], where $P$ is the spatial parity operator, of both quadrupole and octupole deformations are present. One can alternatively use the simplex Hermitian operator $i \exp(-i\tau_j x) P$, where $P$ is the parity operator [14]. I find the use of the operator $S_z$ however much simpler to implement numerically, particularly if one uses a coordinate representation of the quasiparticle wave functions on spatial 3D lattice, see Section VI. If one uses the operator $S_z$, then quasiparticle states with $\eta = \text{sign}(m) = \pm 1$ are assigned to particle numbers $N_\pm$ and densities $n_\pm(r, \sigma, \sigma')$ respectively.

Another option would be to use the operator $i \exp(-i\tau_j x) = i \exp(-i m \pi) = \pm 1$. In this case quasiparticle states with $m = +1/2, -3/2, +5/2, \ldots$ are assigned to particle number $N_+$ and $n_+(r, \sigma, \sigma')$, and states with $m = -1/2, +3/2, -5/2, \ldots$ are assigned to particle number $N_-$ and $n_-(r, \sigma, \sigma')$, respectively. Time-reversed partners are in both cases assigned to different groups, but using different criteria. Since nuclear energy density functionals typically depend on $n(r, \sigma, \sigma') = n_+(r, \sigma, \sigma') + n_-(r, \sigma, \sigma')$ this ambiguity is likely immaterial, unless the nucleus is in the presence of a strong external field, e.g. in magnetars.

This ambiguity in assigning the quasiparticle states to either one or another partial number density in the case of an odd fermion number is general. One can use any rule to separate quasiparticle states in two groups, and there is no general prescription on how to assign them to specific particle number or number densities. The best solution should always correspond to the lowest total energy, which might not always favor the strongest pairing correlations. The many-fermion self-consistent equations never have a unique solution, even for even or even-even systems, though only one of them is the lowest total energy. Multiple vacua however, can also correspond to physically realizable states, separated by strong potential barrier, a situation which is quite ubiquitous in quantum field theories or infinite many-body systems, where symmetry is spontaneously broken. The ambiguities I discuss

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2 The operator $R_x = \exp(-i\tau_j x) = -R_0^2$ is anti-Hermitian, since $R_0^2 R_x = 1$ and $R_0^2 = -1$ for a fermions state.
here for odd fermion systems in this sense should not come as a surprise, but merely as new examples of such physically realizable “ground states.” However, since in the case of odd fermion systems the density of low energy levels is relatively high, any such prescription is to some extent arbitrary, and the true ground state might emerge as an optimal superposition of many such quasi-particle vacua, with well defined quantum numbers. One of the simplest examples is that of a system with spontaneous parity breaking, when the ground and the first excited states are separated by an exponentially small energy difference, a phenomenon known in the literature as parity doubling [19, 20]. Another possibility is that of shape coexistence, see e.g. Refs. [21, 22] and references therein, of which there are many examples of other types too.

There is still another ambiguity. If both quadrupole and octupole deformations are present in a nucleus with axial symmetry, it is not clear whether the ground state of the nucleus corresponds to either $N_+ - N_- = \pm 1$, and thus whether the projection of the total angular momentum $j_z(n) = \sum_{n=1}^N j_z(n)$ is along or opposite to the fission direction. Such a situation can be experimentally studied in fission induced by a nucleon transfer from an impinging projectile to a nucleon state with relatively large angular momentum [23]. The projectile will impact an angular momenta perpendicular to the reaction plane equal to either $\pm m \approx \pm R k_F$, where $R$ is the radius of the target and $k_F$ is its Fermi momentum. The emergence of the fission fragments emitted along the axis perpendicular to the reaction plane, might favor the emission of the either the light or of the heavy fission fragment in the direction of the impacted angular momentum. It would very interesting to see if any asymmetry of the fission fragments distribution along the direction perpendicular to the reaction plane exists, as such a phenomenon has not been studied yet to my knowledge.

IV. THE CASE OF FERMIONIC POLARIZED COLD ATOM SYSTEMS

In the case of cold atoms one has two flavors of fermions, which I shall denote with $a$ and $b$, and the Cooper pair is formed between one fermion $a$ with another fermion $b$. Entangled states, when for example a type $a$ fermion can coexist with a type $b$ fermion, in a type of the Schrödinger cat single-particle state, have not been studied yet, neither experimentally nor theoretically to my knowledge. Only the formation of Cooper pairs between a type $a$ fermion and a type $b$ fermion have been considered so far in the literature. Such a mixing is formally similar to the spin-orbit coupling of the nucleon motion in nuclei, and it will be illustrated qualitatively in Fig. 1. In the absence of such mixing the mean field equations read [4–7, 12]:

$$
\begin{pmatrix}
H_a - \mu_a & 0 & 0 & \Delta \\
0 & H_b - \mu_b & -\Delta & 0 \\
0 & -\Delta^* & -H_a^* + \mu_a & 0 \\
\Delta^* & 0 & 0 & -H_b^* + \mu_b
\end{pmatrix}
\begin{pmatrix}
u_k^{(a)} \\
u_k^{(b)} \\
u_k^{(a)} \\
u_k^{(b)}
\end{pmatrix}
= \mathcal{H}
\begin{pmatrix}
u_k^{(a)} \\
u_k^{(b)} \\
u_k^{(a)} \\
u_k^{(b)}
\end{pmatrix}
= E_k
\begin{pmatrix}
u_k^{(a)} \\
u_k^{(b)} \\
u_k^{(a)} \\
u_k^{(b)}
\end{pmatrix},
$$

where the two chemical potentials $\mu_{a,b}$ are chosen by fixing the particle numbers

$$
N_{a,b} = \sum_{E_k > 0} \int d^3r |\psi_k^{(a,b)}(r)|^2.
$$

![Image](image_url)

**FIG. 1.** The quasiparticle spectrum $E_{k,\pm}^{(a)}$ (31) with blue and $E_{k,\pm}^{(b)}$ (32) with red lines respectively. The densities are constructed from quasi-particle states with $E_{k,\pm}^{(a,b)} > 0$ only. For a finite polarization the quasi-particle states corresponding to the red line with $E_k^{(b)} > 0$. At the same time the fermions of kind $a$ occupy quasi-particle states corresponding to the blue lines with $E_{k,\pm}^{(a)} > 0$. The effect of a non-vanishing mixing between the two flavors or of a spin-orbit coupling (characteristic to nuclear systems) on the quasi-particle spectrum is illustrated with dashed lines. In the case of cold atoms this type of mixing is equivalent to the creation of a Schrödinger cat fermion state between type $a$ and type $b$ flavors.

These equations obviously decouple and since in case of cold atoms one typically has $H_{a,b} = H_{a,b}^*$ the equations simplify. By introducing

$$
H_k = \frac{H_a + H_b}{2}
$$

(27)
these equations can be re-written as
\[
\begin{pmatrix}
H_{+} - \mu & \Delta \\
\Delta^* & -H_{+} + \mu
\end{pmatrix}
\begin{pmatrix}
\eta_k^{(a)} \\
\eta_k^{(b)}
\end{pmatrix}
= \begin{pmatrix}
E_k^{(a)} - \left( H_{+} - \mu \right) & 0 \\
0 & E_k^{(b)} - \left( H_{-} - \mu \right)
\end{pmatrix}
\begin{pmatrix}
\eta_k^{(a)} \\
\eta_k^{(b)}
\end{pmatrix},
\]
(28)

\[
\begin{pmatrix}
H_{+} - \mu & -\Delta \\
-\Delta^* & -H_{+} + \mu
\end{pmatrix}
\begin{pmatrix}
\eta_k^{(a)} \\
\eta_k^{(b)}
\end{pmatrix}
= \begin{pmatrix}
E_k^{(a)} - \left( H_{+} - \mu \right) & 0 \\
0 & E_k^{(b)} + \left( H_{-} - \mu \right)
\end{pmatrix}
\begin{pmatrix}
\eta_k^{(a)} \\
\eta_k^{(b)}
\end{pmatrix},
\]
(29)

and now one can disentangle the different roles operators
\( H_{+} - \mu \) and \( H_{-} - \mu \) play on acting on quasiparticle wave functions. The chemical potentials \( \mu \) and \( \mu \eta \) are defined in a similar manner
\[
\mu = \frac{\mu_a + \mu_b}{2}, \quad \mu \eta = \frac{\mu_a - \mu_b}{2}.
\]
(30)

The self-consistent equations in the nuclear case can be brought to a similar form. Assuming that \( H_{a,b} = \varepsilon_{a,b} \) and \( \Delta \) are diagonal one can show that
\[
E_{k,\pm}^{(a)} = \varepsilon_{a} \pm \sqrt{\varepsilon_{a}^2 + |\Delta|^2},
\]
(31)
\[
E_{k,\pm}^{(b)} = \varepsilon_{b} \pm \sqrt{\varepsilon_{b}^2 + |\Delta|^2},
\]
(32)
\[
\varepsilon_{\pm} = \frac{\varepsilon_{a} - \varepsilon_{b}}{2} - \mu, \quad \varepsilon_k = \frac{\varepsilon_{a} + \varepsilon_{b}}{2} - \mu.
\]
(33)

Clearly all eigenvalues come in pairs \( E_{k,\pm}^{(a)} = -E_{k,\mp}^{(b)} \). For each eigenvector \( (\eta_k^{(a)}, \eta_k^{(b)}) \) and corresponding eigenvalue \( E_{k,\pm}^{(a)} \) of Eq. (28) the Eq. (29) has a corresponding eigenvector \( (\eta_k^{(b)}, \eta_k^{(a)})^* \) and a corresponding eigenvalue \( E_{k,\mp}^{(b)} = -E_{k,\pm}^{(a)} \).

As branches of the quasiparticle spectrum are displaced in opposite directions, when part of the lower branch \( E_{k,\pm}^{(a)} \) becomes positive (with blue in Fig.1) and the upper branch \( E_{k,\pm}^{(b)} \) becomes negative (with red in Fig.1), the roles of the components of the Bogoliubov quasiparticle wave functions change exactly as discussed in Section II, see Eqs. (12, 13). If \( N_a - N_b \) quasiparticle energies \( E_{k,\pm}^{(a)} \) change their signs, then the new quasiparticle vacuum corresponds to \( \prod_{l=1}^{N_a-N_b} \alpha_{l}^{\dagger} \Phi \) and there is a particle parity \((-1)^{N_a-N_b} \) where \( \Phi \) is a total fermion function for an unpolarized system, and \( \mu l \) are the corresponding quantum numbers of the positive \( E_{k,\pm}^{(a)} \) quasiparticle states.

When the branch \( E_{k,\pm}^{(a)} \) and \( E_{k,\pm}^{(b)} \) cross zero, some of the quasiparticles energies could vanish identically, as in the case of bound states on a superfluid vortex line first discussed by Caroli et al. [24] and have a character similar to Majorana particles. In such a case the fermion system is technically a topological one, characterized by a Chern number associated with the Berry connection and curvature [25].

V. MY FAVORITE TWO CHEMICAL POTENTIALS FRAMEWORK FOR A POLARIZED SUPERFLUID FERMI SYSTEM

Likely the best option is to formulate the two chemical potentials framework for nuclei along the same lines as for the scheme suggested for cold atoms, see Refs. [4–7] and Section IV. The main difference between nuclei and cold atom systems is in the presence of the spin-orbit interaction in nuclei and the need to introduce the total single-particle angular momentum \( \hat{l} = \hat{l} + \hat{s} \), where \( \hat{s} = \hat{\sigma}/2 \) is the nucleon spin, and the spin-orbit interaction, which mixes the “spin-ups” and “spin-downs” tates, as discussed in the previous Section IV.

An aspect that is hardly ever discussed in the literature is the choice of the three axes for the spin and their relation with the actual spatial directions. It is easy to verify that the Schrödinger equation for a spin particle is invariant with respect to an arbitrary rotation in the spin space, even in the presence of a spin-orbit interaction, namely
\[
\hat{\sigma} \to \exp \left( \frac{i \psi}{2} \hat{\sigma} \cdot \hat{n} \right) \hat{\sigma} \exp \left( -\frac{i \psi}{2} \hat{\sigma} \cdot \hat{n} \right),
\]
(34)
where \( \hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta) \) is an arbitrary 3D unit vector and \( \hat{\sigma} \) are the Pauli matrices. Basically what this means, that the particular choice of \( \sigma_z \) as a diagonal traceless Hermitian matrix is not unique, and any traceless \( 2 \times 2 \) Hermitian matrix with eigenvalues \( \pm 1 \) is an equally acceptable choice for example. The same applies for the other two Pauli matrices \( \sigma_x, \sigma_y \), with the only requirement that \( [\sigma_k, \sigma_l] = 2i \varepsilon_{klm} \sigma_m \), where
\[
\varepsilon_{klm} = \begin{cases} 1 & \text{if } k,l \text{ are in a } x-y \text{ plane; } m \text{ is } z \text{ axis} \\ -1 & \text{if } k,l \text{ are in a } x-z \text{ plane; } m \text{ is } y \text{ axis} \\ 0 & \text{otherwise} \end{cases}
\]
is the Levi-Civita symbol.

Since \( [\hat{l}, \hat{s}] = 0 \) the rotation operator can be factorized
\[
\exp \left( -i \psi \hat{j} \cdot \hat{n} \right) = \exp( -i \psi \hat{l} ) \exp( -i \psi \hat{s} \cdot \hat{n} ),
\]
(35)
When \( \exp( -i 2 \pi \hat{j} \cdot \hat{n} ) \) is acting on spinor and if the spinor-1/2 wave function changes sign. If one considers now separately the action of \( \exp( -i 2 \pi \hat{l} ) \) on any component of the spinor that component does not change sign. However, when acting with \( \exp( -i 2 \pi \hat{s} \cdot \hat{n} ) \) alone on the entire spinor wave function, the spatial part of the wave function is obviously unaffected, but the whole spinor wave function changes sign. That allows us to define the operator
\[
P_N = \prod_{k=1}^{N} \exp \left[ -i 2 \pi \hat{s}(k) \cdot \hat{n} \right],
\]
(36)
where the product runs over all particles. This operator is nothing else but the particle parity operator \( P_N \Phi = (-1)^N \Phi \) for a fermion system. Since the spin direction can be chosen arbitrarily, one can use \( \hat{n} = (0, 0, 1) \). Since a polarized Fermi system is spin polarized Eqs. (16, 17)
should be rewritten as follows:

\[
\begin{pmatrix}
H_{\eta\uparrow\uparrow} & H_{\eta\uparrow\downarrow} & 0 & \Delta \\
H_{\eta\downarrow\uparrow} & H_{\eta\downarrow\downarrow} & -\Delta & 0 \\
0 & -\Delta^* & -H_{\eta\uparrow\uparrow} & -H_{\eta\uparrow\downarrow} \\
\Delta^* & 0 & -H_{\eta\downarrow\uparrow} & -H_{\eta\downarrow\downarrow}
\end{pmatrix}
\begin{pmatrix}
\langle u_{k,\uparrow}\rangle \\
\langle u_{k,\downarrow}\rangle \\
\langle v_{k,\uparrow}\rangle \\
\langle v_{k,\downarrow}\rangle
\end{pmatrix}
= H \begin{pmatrix}
\langle u_{k,\uparrow}\rangle \\
\langle u_{k,\downarrow}\rangle \\
\langle v_{k,\uparrow}\rangle \\
\langle v_{k,\downarrow}\rangle
\end{pmatrix} = E_k,
\]

(37)

\[
H_{\eta\sigma,\sigma} = H_{\sigma\sigma} - \mu - \eta \mu \eta - Q,
\]

(38)

with \( \eta = \pm 1 \) for \( \uparrow, \downarrow \) respectively. Here I have basically replaced the operator \( S_z \) introduced in Section III with the operator \( i \exp(-i\pi\sigma_z/2) \equiv \sigma_z \). Then the chemical potentials \( \mu_{\uparrow,\downarrow} = \mu \pm \eta \mu \), the number densities, and the particle numbers are determined as follows

\[
n_\sigma(r) = \sum_{km} v_\sigma(r) v_\sigma^*(r,\sigma) \Theta(E_k), \quad \sigma = \uparrow, \downarrow
\]

(39)

\[
n(r) = n_\uparrow(r) + n_\downarrow(r)
\]

(40)

\[
N = N_\uparrow + N_\downarrow, \quad N_{\uparrow,\downarrow} = \int d^3r n_{\uparrow,\downarrow}(r).
\]

(41)

Since the chemical potential \( \mu \eta \) enters in the self-consistent equations Eq. (37) as \( \mu_{\eta\sigma} \) the single-particle angular momentum \( \hat{j}_z \) still commutes with the quasiparticle Hamiltonian \( H \) for an axially symmetric nucleus. However, a spin polarized odd or odd-odd nucleus strictly speaking cannot be spherical anymore in the mean field approximation, as \( [\hat{j}^2, \sigma_z] \neq 0 \).

The quasiparticle spectrum is not affected qualitatively by the presence or absence of the spin-orbit interaction, see Fig. (1). Notice that in these formulas I have dropped the additional subscript \( m \) for the energies and quasiparticle wave functions, as there is no need for singling out \( m \). Various branches of the quasiparticle spectrum are shifted upwards and downwards, see Fig. (1), and the extra quasiparticle state with lowest energy is automatically “flipped,” see Section II.

In the traditional approach used for odd fermion systems, see Refs. [13, 15, 16] and Section II, where the quantum numbers for the singlet out quasiparticle state \( \mu \), see Eq. (11), are a priori unknown, in order to determine the ground state one needs to perform many simulations with various choices of quantum numbers for quasiparticle state \( \mu \). In this latest formulation, c.f. Eqs. (37), one needs only to specify the degree of polarization \( N_\uparrow - N_\downarrow \) of the system only, similarly to what has been done in the case of cold atom systems for arbitrary polarizations, and where the agreement of the density functional approach with ab initio quantum Monte Carlo calculations of inhomogeneous systems and also with experiments was excellent [4, 6, 7, 26, 27]. Notice also that the difficulties with the formulation of the formalism for an fermion system in the case of higher degeneracies, which were discussed in Ref. [8], do not emerge emerge. Moreover, \( N_\uparrow - N_\downarrow \) can take any integer value, a situation which might be very useful when analyzing nuclei, even or odd, in extremely strong magnetic fields, e.g. in magnetars.

### VI. ASPECTS OF NUMERICAL IMPLEMENTATION

If the axial symmetry is codified explicitly into the numerical single-particle basis used, then the action of the operator \( S_z \) discussed in Section III is simply reduced to a multiplication with \( \eta = \text{sign}(m) = \pm 1 \) and levels with positive/negative \( m \) quantum numbers are characterized by different chemical potentials \( \mu_m = \mu \pm \eta \mu \). If instead one uses the operator \( i \exp(-i\pi j_z) \) then \( \eta = i \exp(i\pi m) = \pm 1 \) as well, but the assignment of the quasiparticle states to either \( N \pm \) groups is different, as discussed in Section III. If the time-reversed orbitals with \( +m \) and \( -m \), which are typically involved in the formation of Cooper pairs, when one of them is missing in an odd system this leads to the polarization of the nucleus, as \( n_+(r,\sigma,\sigma') \neq n_-(r,\sigma,\sigma') \).

Numerical implementation of the operators \( S_z i \exp(-i\pi j_z) P, i \exp(-i\pi j_z) P \) on a 3D spatial lattice however can run into numerical inaccuracies, as either the axial symmetry or the rotations can be implemented only approximately. In this respect the use of operator \( S_z \) is preferable, as one can use as an alternative method to determine \( \eta \) the computation of the sign of the expectation value of \( \hat{j}_z \), thus

\[
\eta = \text{sign} \left( \langle v_{km} | \hat{j}_z | v_{km} \rangle \right).
\]

(42)

Therefore this method of introducing the \( \mu \eta S_z \) into the SLDA equation is equivalent to expressing the quasiparticle eigenvalue as an expectation value of the quasiparticle Hamiltonian \( H_{km} \) in the SLDA equations, see Eq. (16), which leads to mathematically equivalent equations.

In the time-dependent problem there is no need to include the operators \( Q \) and \( S_z \) and the simulation will run as usual, even when symmetries are broken during evolution.

The presence of an odd fermion on top of an even core leads to the density polarization of the even fermion core and also can lead to time-reversal symmetry breaking in the ground state of such a system. The determination of the eigenvalues and of the eigenvectors of Eq. (37) when many/all symmetries are broken and particularly for the

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3 |\( N_\uparrow - N_\downarrow \) could be any integer in principle and therefore in this framework one can generate two or more quasiparticle excited states as well if needed.
needs of time-dependent simulations, is an extremely computationally demanding problem. This problem is significantly simplified by noticing that the stationary solution is determined fully by the densities alone, and the explicit presence of quasiparticle wave functions is not required. The costly quasiparticle Hamiltonian diagonalization can then be replaced by a significantly faster algorithm, either the shifted conjugate orthogonal conjugate gradient method [28] or the conjugate orthogonal conjugate residual method [29]. As during the iterative process the lowest quasiparticle particle levels change their positions, sometimes quite dramatically and their ordering can be significantly modified, a simulated annealing method in conjunction with the iterative process can lead to a significant stabilization of the iterations and the need to specify in advance a specific quasiparticle state \( \mu \) is then eschewed. Within a simulated annealing process the iterative process starts at a finite temperature, which is lowered according to a predetermined schedule, and as the iterative process starts converging, eventually the temperature reaches the goal \( T = 0 \) (\( T \) is the temperature). Figuratively, the black zero energy line in Fig. 1 gets blurred and acquires a finite width \( \sim O(T) \). In this manner quasiparticle states with both positive and negative energies \( E_k \) in a narrow energy band \( |E_k| \sim O(T) \) contribute to the densities and the somewhat erratic behavior of low energy quasiparticle energies during the iterative process is mitigated. The simulated annealing method has been applied successfully to cold atom systems [4–12]. The iterative process can likely be further accelerated also by using the gradient method advocated by Robledo and Bertsch [17], which to be used in conjunction with the methods proposed by Jin et al. [28] and Kashiwaba and Nakatsuksa [29]. After the iterative process converged one has to perform only a single diagonalization in order to determine the quasiparticle wave functions, which are needed as input for time-dependent simulations [2, 3, 30–34].

VII. CONCLUSIONS

I discussed here several frameworks suggested in the literature, as well as a few new ones, designed to treat odd fermion superfluid systems, their advantages and disadvantages, and I introduced a two chemical potential framework, which appears to me to be superior to the suggested so far in the literature frameworks. Unlike the general framework designed by Dobaczewski and Dudek [13], which requires an \( a \) priori knowledge of the quantum numbers characterizing the odd extra fermion, the two chemical potentials framework introduced here and outlined in Section V, when properly numerically formulated, see Section VI, eschews the diagonalization of the quasiparticle Hamiltonian, used in order to arrive at a self-consistent solution, and also the need to \( a \) priori identify the quantum numbers of the extra fermion, as the contribution of the lowest energy quasiparticle state of the odd fermion is automatically selected in this framework, particularly when the simulated annealing method is also incorporated in the iterative process. The gradient method advocated by Robledo and Bertsch [17] apparently also does not require the \( a \) priori identification of the quantum numbers of the odd fermion. At this time it is not clear whether either the simulated annealing method or the gradient method for generating the new mean field during the iterative process is superior computationally, or even if a carefully combination of the simulated annealing with the gradient method could prove to be the best choice. Since there exists methods [28, 29], which eschew the ubiquitous diagonalization of the quasiparticle Hamiltonian used routinely in the literature, in conjunction with simulated annealing and/or gradient methods, in the mean field calculations of polarized fermion systems one can achieve a significant numerical speed-up. The framework describe here can be particularly useful to describe nuclei in the presence of extremely strong magnetic fields, encountered in magnetars for example.

I have conjectured that by studying the asymmetry of the fission fragments distributions, emitted along the direction of the angular momentum of the fissioning odd or odd-odd nucleus one could shed new light on whether low energy quasiparticle components play a qualitative new role in fission. Compound states in fissioning nuclei with relatively large angular momenta can be populated in neutron pick-up reactions [23]. Similar, but not identical, type of correlations have been recently analyzed within the phenomenological model CGMF [35] based on the Hauser-Feshbach framework [36] by Lovell et al. [37] in neutron induced fission of actinides. These authors, while pointing to quite a number of experimental results, observe that with the increasing energy of the incident neutron the anisotropy for the reaction \( \text{U}^{235}(n,f) \) is noticeably more pronounced than for the reactions \( \text{U}^{235}(n,f) \) and \( \text{Pu}^{239}(n,f) \). This analysis thus suggests that fission is favored along the direction of the total angular momentum of the compound nucleus. This type of anisotropy has been postulated by Bohr [38]. It is not clear yet however, whether the emission of the heavy fission fragment is favored or hindered over the emission of the light fission fragment along the direction of the total angular momentum of the compound nucleus.

VIII. ACKNOWLEDGEMENT

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\[ \text{Unfortunatel I could not provide a more complete reference to this source due to the inability to use a library at this time.} \]
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