DENSITY MATRIX FUNCTIONAL THEORY
WITH ACCOUNT OF PAIRING CORRELATIONS

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Abstract

The extension of the density functional theory (DFT) to include pairing correlations without formal violation of the particle-number conservation condition is described. This version of the theory can be considered as a foundation of the application of existing DFT plus pairing approaches to atoms, molecules, ultracooled and magnetically trapped atomic Fermi gases, and atomic nuclei where the number of particles is exactly conserved. The connection with the Hartree-Fock-Bogoliubov theory is discussed. The method of the quasilocal reduction of the nonlocal theory is described. This quasilocal reduction allows to obtain equations of motion which are much more simple for the numerical solution than the equations corresponding to the nonlocal case.

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1 INTRODUCTION

Although both the theory of superconductivity and the density functional theory (DFT) have a long history, models which take into account pairing correlations within the framework of the DFT have appeared not so long ago. The initial version of the DFT developed in the early papers of Hohenberg, Kohn, and Sham [1, 2] did not include the pairing correlations explicitly. The first generalization of the DFT in this direction was developed in Ref. [3] for superconductors. However, the essential feature of this theory is the nonconservation of the number of particles in the superconducting Fermi system. Consequently, the application of the DFT for superconductors to atoms, molecules, ultracooled and magnetically trapped atomic Fermi gases, and atomic nuclei, where the pairing correlations may be important but the number of particles is exactly conserved, requires an additional foundation. In fact, the same question emerges in connection with the DFT plus pairing approaches based, for example, on the theory of finite Fermi systems of Migdal (see [4] and references therein) or on the local density approximation (Ref. [5]). So the first goal of the present paper is a rigorous formulation of the extended version of the DFT taking into account the pairing correlations under the condition of particle-number conservation.

The second goal is to extend the DFT to the case of a functional dependence on the total nonlocal single-particle density matrix (DM). Such an extension is especially important in applications to nuclei because it allows to introduce in a natural way the kinetic-energy and the spin densities dependence of the energy functional. That kind of dependence leads to the appearance of a radial-dependent effective mass and a spin-orbit potential which are essential components of the nuclear structure models. Let us note that the original version of the DFT can be classed as a local theory because in the papers [1, 2] the energy functional only depends on the local particle density. One of the possible ways of a nonlocal extension of the DFT was considered in Ref. [6]. However, this method, which can be referred to as a straightforward extension, faces with serious difficulties related with the equations of motion and their physical interpretation. Another method has been recently developed in Ref. [7] to extend the DFT by considering an energy functional which depends on a Slater-determinant DM. This approach leads to the quasilocal density functional theory and allows to avoid the difficulties arising from the method described in [6] but, in general, the resulting DM is not the exact DM because only its diagonal part is the quantity which coincides with the exact local particle density of the interacting fermion system.
In the present paper we will show that the inclusion of the pairing within the framework of the extended DFT is enough to obtain the exact total nonlocal DM on the one hand, and to avoid the difficulties encountered in the equations of motion of Ref. [6] on the other hand. Although we develop our formalism in the particular case of atomic nucleus, the main results and conclusions can also be applied to any Fermi system with a fixed number of particles. The paper is organized as follows. In Sec. 2 the extended density matrix (EDM) formalism is revised. In Sec. 3 the DFT is extended in order to include the pairing correlations. In Sec. 4 the reduction to an extended quasilocal density functional theory is performed. The conclusions are given in the last section. In the Appendices some mathematical details and comments are presented.

2 EXTENDED DENSITY MATRIX FORMALISM

Despite the formalism of the density matrix extended to include pairing correlations in the ground state is well known (see, e. g., Refs. [8, 9]), we shall draw some basic definitions which are necessary for the further analysis. Let Ψ be some arbitrary antisymmetrized many-fermion wave function. In the general case Ψ is assumed to be normalized, but it is not supposed to be an eigenfunction of the particle-number operator. Thus the normal (ρ) and the anomalous (κ) density matrices in the state Ψ are defined through the following expectation values:

\[ \rho(x,x') = \langle \Psi | a^\dagger(x') a(x) | \Psi \rangle, \]  

\[ \kappa(x,x') = \langle \Psi | a(x') a(x) | \Psi \rangle, \quad \kappa^*(x,x') = \langle \Psi | a^\dagger(x) a^\dagger(x') | \Psi \rangle, \]  

where \( a^\dagger(x) \) and \( a(x) \) are creation and annihilation operators of particles in the coordinate representation of the usual single-particle space. In the case of atomic nuclei, symbol \( x = \{r, \sigma, q\} \) includes the spatial coordinate \( r \) and the spin projection \( \sigma \) variables as well as the index \( q = n, p \) indicating the nucleon type (neutrons and protons).

It is important to note that for Fermi systems, which are considered here, the ground state (GS) is described by a wave function \( \Psi = \Psi_{GS} \) with a fixed number of particles. Therefore, in the GS the anomalous DM vanishes:

\[ \kappa_{GS}(x,x') = 0. \]  

However, in many physical problems one can construct auxiliary quantities, which have the
sense of an anomalous DM but nevertheless take nonzero values in the GS even if the Eq. (3) is fulfilled.

Let us suppose that the DM \( \rho \) defined by Eq. (1) is given for some wave function \( \Psi \) (in particular, it may be the exact GS wave function \( \Psi_{\text{GS}} \)). If \( \Psi \) is time-reversal invariant, we can introduce the canonical basis (CB) \( \{ \phi_\lambda(x) \} \), where the single-particle multiindex \( \lambda \) contains the sign of the spin projection \( s \) and the set of the remaining quantum numbers \( \{ c \} \) (\( \lambda = \{ c, s \} \)), so that the following expansion is fulfilled

\[
\rho(x, x') = \sum_{c,s} v^2_c \phi_{c,s}(x) \phi^*_{c,s}(x'), \quad 0 \leq v_c \leq 1.
\]

(4)

In the case of real Fermi systems, this DM is not idempotent (i.e. \( \rho^2 \neq \rho \)). This is due to the fact that all or almost all the eigenvalues of \( \rho \), defined by the equation \( \int dx' \rho(x, x') \phi_{c,s}(x') = v^2_c \phi_{c,s}(x) \) (hereinafter \( \int dx \) means the space integral over \( r \) and the sum over \( \sigma \) and \( q \) indices), lie in the interval \( 0 < v^2_c < 1 \). If one uses, as it was done in the theory developed by Gilbert in Ref. [6], an energy functional \( E_G[\rho] \) depending only on such nonlocal and non-idempotent DM, in the resulting equations of motion all partially occupied natural spin orbitals (i.e. functions \( \phi_{c,s}(x) \) for which \( 0 < v^2_c < 1 \)) are eigenfunctions of the single-particle pseudo-Hamiltonian \( h_G(x, x') = \delta E_G[\rho]/\delta \rho(x', x) \) with the same eigenvalue (see Ref. [6] for details). This fact leads to difficulties in the physical interpretation and in the mathematical foundation of the theory developed by Gilbert. To avoid this problem, first of all we shall define an extended density matrix (EDM) \( \mathcal{R} \) which has to be idempotent \( (\mathcal{R}^2 = \mathcal{R}) \) on the one hand and has to contain a given DM \( \rho \) as a block on the other hand. An EDM means a DM which is defined in a space being the doubled usual single-particle space.

Let \( \{ \psi_{\lambda,\eta}(x; \chi) \} \) be an arbitrary set of basis functions in this extended space spanned by the coordinates \( \{ x, \chi \} \), where \( \chi = \pm 1 \) and \( \eta = \pm 1 \) are additional indices introduced for denoting the different components of the single-particle functions. The meaning of these indices will be specified in the following (in particular, the index \( \chi \) indicates the upper and lower components of the functions \( \psi_{\lambda,\eta}(x; \chi) \) according to notations of Ref. [9]). The usual conditions of orthonormality and completeness are supposed to be satisfied:

\[
\sum_{\lambda} \int dx \psi^*_{\lambda,\eta}(x; \chi) \psi_{\lambda',\eta'}(x; \chi) = \delta_{\eta,\eta'} \delta_{\lambda,\lambda'}, \quad (5)
\]

\[
\sum_{\lambda,\eta} \psi^*_{\lambda,\eta}(x; \chi) \psi_{\lambda',\eta}(x' ; \chi') = \delta_{\chi,\chi'} \delta(x, x'), \quad (6)
\]

where \( \delta(x, x') = \delta(r - r') \delta_{\sigma,\sigma'} \delta_{q,q'} \). In addition we also assume that the functions \( \psi_{\lambda,\eta}(x; \chi) \)
satisfy the condition:

\[ \psi_{\lambda;\eta}(x;\chi) = \psi_{\lambda;\eta}^*(x;-\chi) . \]  

From the conditions (5) and (6) it follows that the functions \( \psi_{\lambda;\eta}(x;\chi) \) form a unitary matrix in the extended space defined previously. (Strictly speaking, they form a unitary operator. The use of the term matrix implies that the configuration space is discretized and restricted by a finite number of points.) If the condition (7) is also fulfilled, the Bloch-Messiah theorem (see Refs. [8] [10]) can be applied to this matrix. In order to reformulate this theorem in coordinate representation let us first introduce a complete set of orthonormal functions \( \{ \tilde{\phi}_\lambda(x) \} \). Notice that these functions form a unitary matrix \( D \) in the notation of Ref. [8] according to the rule: \( D_{i,k} = \tilde{\phi}_\lambda(x_i) \). Second, let us divide the set of the single-particle indices \( \lambda \) into three subsets: two sets of conjugate indices \( p \) and \( \bar{p} \) which represent “paired” states and the set of the indices \( b \) corresponding to “blocked” states, i.e.: \( \{ \lambda \} = \{ p \} \cup \{ \bar{p} \} \cup \{ b \} \). Let, further, \( \bar{v}_\lambda \) and \( \bar{u}_\lambda \) be real non-negative numbers which satisfy the following conditions: \( \bar{u}_\lambda = \sqrt{1 - \bar{v}_\lambda^2} \), \( \bar{v}_p = \bar{v}_{\bar{p}} \), \( 0 < \bar{v}_p < 1 \), \( \bar{v}_b^2 = \bar{v}_b \). According to the Bloch-Messiah theorem the functions \( \psi_{\lambda;\eta}(x;\chi) \) can be represented in the following form

\[ \psi_{\lambda;+}(x;\chi) = \sum_{\lambda'} C_{\lambda\lambda'} \tilde{\psi}_{\lambda';+}(x;\chi) , \quad \psi_{\lambda;-}(x;\chi) = \sum_{\lambda'} C_{\lambda\lambda'} \tilde{\psi}_{\lambda';-}(x;\chi) , \]  

(8)

where \( C_{\lambda\lambda'} \) is a unitary matrix, and the functions \( \tilde{\psi}_{\lambda;\eta}(x;\chi) \) have the form:

\[
\begin{align*}
\tilde{\psi}_{p;+}(x;+) &= \bar{u}_p \tilde{\phi}_p(x) , & \tilde{\psi}_{\bar{p};+}(x;+) &= \bar{u}_{\bar{p}} \tilde{\phi}_{\bar{p}}(x) , & \tilde{\psi}_{b;+}(x;+) &= \bar{u}_b \tilde{\phi}_b(x) , \\
\tilde{\psi}_{p;+}(x;-) &= -\bar{v}_p \tilde{\phi}_p(x) , & \tilde{\psi}_{\bar{p};+}(x;-) &= \bar{v}_{\bar{p}} \tilde{\phi}_{\bar{p}}(x) , & \tilde{\psi}_{b;+}(x;-) &= \bar{v}_b \tilde{\phi}_b(x) , \\
\tilde{\psi}_{p;+}(x;+)' &= \bar{u}_p \tilde{\phi}_p(x) , & \tilde{\psi}_{\bar{p};+}(x;+)' &= \bar{u}_{\bar{p}} \tilde{\phi}_{\bar{p}}(x) , & \tilde{\psi}_{b;+}(x;+)' &= \bar{u}_b \tilde{\phi}_b(x) , \\
\tilde{\psi}_{p;+}(x;-)' &= \bar{u}_p \tilde{\phi}_p(x) , & \tilde{\psi}_{\bar{p};+}(x;-)' &= \bar{u}_{\bar{p}} \tilde{\phi}_{\bar{p}}(x) , & \tilde{\psi}_{b;+}(x;-)' &= \bar{u}_b \tilde{\phi}_b(x) ,
\end{align*}
\]

(9)

Let us now define the EDM \( \mathcal{R} \) in terms of the arbitrary set of functions \( \{ \psi_{\lambda;\eta}(x;\chi) \} \) introduced above by the formula

\[ \mathcal{R}(x,\chi; x',\chi') = \sum_{\lambda} \psi_{\lambda;-}(x;\chi) \psi_{\lambda;-}^*(x';\chi') . \]  

(10)

Using Eqs. (5) – (7) it can be easily shown that the following equalities are fulfilled:

\[ \mathcal{R}^2 = \mathcal{R} , \quad \mathcal{R}^\dagger = \mathcal{R} , \]  

(11)

\[ \mathcal{R}(x,\chi; x',\chi') = \delta_{\chi,\chi'} \delta(x, x') - \mathcal{R}(x',-\chi'; x,-\chi) . \]  

(12)
Let us introduce notations for the blocks of the EDM taking into account the properties (11) – (12):

\[
\begin{align*}
R(x, + ; x', +) &= \tilde{\rho}(x, x'), \\
R(x, + ; x', -) &= \tilde{\kappa}(x, x'), \\
R(x, - ; x', +) &= -\tilde{\kappa}^*(x, x'), \\
R(x, - ; x', -) &= \delta(x, x') - \tilde{\rho}^*(x, x'),
\end{align*}
\tag{13}
\] or in the matrix representation:

\[
R = \begin{pmatrix}
\tilde{\rho} & \tilde{\kappa} \\
-\tilde{\kappa}^* & 1 - \tilde{\rho}^*
\end{pmatrix}.
\tag{14}
\]

As it will be clear in the following (see Eqs. (21) – (22) below), the blocks \(\tilde{\rho}\) and \(\tilde{\kappa}\) play the role of the normal and anomalous density matrices in some (quasi-particle vacuum) state.

Substituting Eqs. (8) and (9) into Eq. (10), we obtain:

\[
\tilde{\rho}(x, x') = \sum_{\lambda} \tilde{v}_{\lambda}^2 \bar{\phi}_\lambda(x) \bar{\phi}_\lambda^*(x'),
\tag{15}
\]

where the sum over \(\lambda\) implies the sum over the three sets of indices \(p, \bar{p},\) and \(b\). Thus, the functions \(\tilde{\phi}_\lambda(x)\) form the CB in which \(\tilde{\rho}(x, x')\) is diagonal. So in the following we shall refer to Eqs. (9) as the CB representation of the functions \(\psi_{\lambda\eta}(x; \chi)\).

Comparing Eqs. (4) and (15) we see that the expansion (4) is a particular case of (15). Indeed, setting the number of blocked occupied states in (15) to be even or to be equal to zero, one can choose \(\tilde{v}_{\lambda} = v_{\lambda}, \bar{\phi}_\lambda(x) = \phi_\lambda(x)\), which leads to the coincidence of the right-hand sides of Eqs. (4) and (15). So, there exists a variety of sets of the functions \(\psi_{\lambda\eta}(x; \chi)\), which enter into the definition (10) and differ by an arbitrary unitary transformation of the type Eq. (8), such that the following equalities are fulfilled:

\[
R(x, + ; x', +) = \tilde{\rho}(x, x') = \rho(x, x').
\tag{16}
\]

Due to the fact that Eq. (4) is fulfilled for any physically meaningful DM \(\rho\), actually we have proved that for an arbitrary nonlocal DM \(\rho(x, x')\), corresponding to some interacting time-reversal invariant fermion system, we can construct an EDM \(R\) which satisfies the conditions (11) – (12) and which is related with the DM \(\rho\) by the formula (16).

It is important to note that, if the normal DM \(\rho\) is produced by some wave function \(\Psi\) according to Eq. (1), the anomalous DM \(\kappa\) produced by the same wave function \(\Psi\) according to Eqs. (2) does not coincide, in general, with the quantity \(\tilde{\kappa}\) defined as a block of the EDM by Eqs. (13), even if Eqs. (16) are fulfilled. In particular, if \(\Psi = \Psi_{\text{GS}}\) then, as it was
mentioned above, \( \kappa = \kappa_{\text{GS}} = 0 \), but for the interacting system \( \tilde{\kappa} \neq 0 \). On the other hand, if \( \Psi \) is a quasiparticle-vacuum wave function (see below), then the equality \( \kappa = \tilde{\kappa} \) is fulfilled.

In order to reproduce an arbitrarily given DM \( \rho(x,x') \) as a block of the EDM \( \mathcal{R} \) we have started from an arbitrary complete set of basis functions \( \{ \psi_{\lambda}(x;\chi) \} \) which satisfies the conditions (5) – (7). It is useful to do it in a different way, looking at this problem from another more traditional point of view. To this end, let us introduce the creation and annihilation operators of the quasiparticles \( \alpha_{\lambda}^\dagger \) and \( \alpha_{\lambda} \) through the equation:

\[
\left( \begin{array}{c}
\alpha_{\lambda}^\dagger \\
\alpha_{\lambda}
\end{array} \right) = \int dx \left( \begin{array}{cc}
\psi_{\lambda,+}(x;+) & \psi_{\lambda,+}(x;-) \\
\psi_{\lambda,-}(x;+) & \psi_{\lambda,-}(x;-)
\end{array} \right) \left( \begin{array}{c}
a^\dagger(x) \\
a(x)
\end{array} \right).
\] (17)

With this definition the functions \( \psi_{\lambda}(x;\chi) \) form the matrix of the Bogoliubov transformation. Then the properties (5) – (7) simply follow from the requirement of the unitarity of this transformation and from the fact that \( \alpha_{\lambda}^\dagger \) and \( \alpha_{\lambda} \) are a Hermitian conjugate pair of the operators. The inverse relation, which follows from (6) and (7), reads:

\[
\left( \begin{array}{c}
a^\dagger(x) \\
a(x)
\end{array} \right) = \sum_{\lambda} \left( \begin{array}{cc}
\psi_{\lambda,-}(x;-) & \psi_{\lambda,+}(x;-) \\
\psi_{\lambda,-}(x;+) & \psi_{\lambda,+}(x;+)
\end{array} \right) \left( \begin{array}{c}
\alpha_{\lambda}^\dagger \\
\alpha_{\lambda}
\end{array} \right).
\] (18)

Let us define the quasiparticle-vacuum wave function \( \tilde{\Psi} \) by the ordinary condition:

\[
\alpha_{\lambda} |\tilde{\Psi}\rangle = 0, \quad \forall \lambda.
\] (19)

This definition is unique, and the wave function \( \tilde{\Psi} \) defined by the condition (19) is invariant under the \( C \)-transformation (8). So, one can find the explicit general form of \( \tilde{\Psi} \) by using the CB representation (9). The result is well known (see, e. g., Ref. [8]) and reads:

\[
|\tilde{\Psi}\rangle = \prod_{b}(\bar{\upsilon}_b + \bar{\upsilon}_b \alpha_b^\dagger) \prod_p(\bar{\upsilon}_p + \bar{\upsilon}_p \alpha_p^\dagger \alpha_{\bar{p}}^\dagger) |0\rangle,
\] (20)

where \( |0\rangle \) is the particle-vacuum wave function, \( \alpha_{\lambda}^\dagger = \int dx \tilde{\phi}_{\lambda}(x) a^\dagger(x) \). If, further, we formally define the EDM \( \mathcal{R} \) through Eqs. (13) with

\[
\tilde{\rho}(x,x') = \langle \tilde{\Psi} | a(x') a(x) |\tilde{\Psi}\rangle,
\] (21)

\[
\tilde{\kappa}(x,x') = \langle \tilde{\Psi} | a(x') a(x) |\tilde{\Psi}\rangle, \quad \tilde{\kappa}^*(x,x') = \langle \tilde{\Psi} | a^\dagger(x) a^\dagger(x') |\tilde{\Psi}\rangle,
\] (22)

then it is easy to show using Eqs. (18) and (19) that this EDM is expressed in terms of the functions \( \psi_{\lambda}(x;\chi) \) by Eq. (10), and consequently it satisfies Eqs. (11) – (12). In other
words, Eqs. (13), (21), (22) set a mapping of $\tilde{\Psi}$ onto the EDM $\mathcal{R}$ satisfying Eqs. (10) – (12). In the following the many-to-one mappings of the many-fermion wave functions (e. g., $\tilde{\Psi}$) to the density matrices (e. g., $\tilde{\rho}$ or $\mathcal{R}$), defined by equations of the type (13), (21), and (22), will be denoted as $\tilde{\Psi} \to \tilde{\rho}$ or $\tilde{\Psi} \to \mathcal{R}$. Due to the fact that in the above derivation the matrix elements of the Bogoliubov transformation $\psi_{\lambda;\eta}(x;\chi)$ are constrained only by conditions (5) – (7), the existence of the pointed mapping $\tilde{\Psi} \to \mathcal{R}$ is true, in particular, if $\psi_{\lambda;\eta}(x;\chi)$ are chosen in such a way that Eqs. (16) are fulfilled for some arbitrarily given DM $\rho$ (that is always possible as was proved above). Then we have also the mapping $\tilde{\Psi} \to \mathcal{R} \to \rho$. Consequently, it can be argued that for an arbitrary nonlocal DM $\rho(x,x')$, corresponding to some interacting time-reversal invariant fermion system, including the case for which the number of particles is exactly conserved, there exists a quasiparticle-vacuum wave function $\tilde{\Psi}$ such that $\tilde{\Psi} \to \rho$. The explicit form of $\tilde{\Psi}$ is given by Eq. (20), in which $\tilde{v}_\lambda$ and $\tilde{\phi}_\lambda(x)$ are the eigenvalues ($v_\lambda^2$) and the eigenfunctions ($\phi_\lambda(x)$) of the given DM $\rho$. The opposite is also true: any quasiparticle-vacuum wave function, which satisfies the condition $\tilde{\Psi} \to \rho$, has the general explicit form (20) with $\tilde{u}_\lambda = u_\lambda$, $\tilde{v}_\lambda = v_\lambda$, $\tilde{\phi}_\lambda(x) = \phi_\lambda(x)$.

These statements can be considered as a generalization of the Lieb theorem [11] proved for the local particle density and the Slater-determinant wave functions. It is remarkable that the inclusion of the pairing is enough not only to prove a more general statement but also to make the proof much more simple. Moreover, the proof of Lieb is based on the particular example of a Slater-determinant wave function which produces a given local particle density. However, in the Lieb theorem the general explicit form of such Slater-determinant wave function is not constructed. In contrast, in our case the general explicit form (20) of the quasiparticle-vacuum wave function, which satisfies the condition $\tilde{\Psi} \to \rho$, is known.

3 EXTENSION OF THE DFT

Let $H$ be the nonrelativistic exact many-body Hamiltonian of an interacting fermion system. Let us define an auxiliary functional which depends only on the normal nonlocal DM $\rho$:

$$E[\rho] = \inf_{\Psi \to \rho} \langle \Psi | H | \Psi \rangle,$$

(23)

where $\Psi$ are arbitrary normalized many-fermion wave functions, including the ones with a fixed number of particles. Following the method of Ref. [7] let us introduce an effective
many-body Hamiltonian $\tilde{H}$ which generally does not coincide with $H$. Now we define

$$\tilde{E}[\rho, \tilde{\kappa}, \tilde{\kappa}^*] = \inf_{\tilde{\Psi} \rightarrow \rho, \tilde{\kappa}, \tilde{\kappa}^*} \langle \tilde{\Psi} | \tilde{H} | \tilde{\Psi} \rangle ,$$

(24)

where $\tilde{\Psi}$ are the quasiparticle-vacuum wave functions. Due to the existence of the mapping $\tilde{\Psi} \rightarrow \rho$ proved in the previous section, the functional $\tilde{E}[\rho, \tilde{\kappa}, \tilde{\kappa}^*]$ can be defined for an arbitrary nonlocal DM $\rho(x,x')$ corresponding to some interacting time-reversal invariant fermion system with a fixed number of particles and for those matrices $\tilde{\kappa}, \tilde{\kappa}^*$ which are produced by the quasiparticle-vacuum wave functions according to Eqs. (22). Notice, however, that Eq. (24) implies that $\tilde{H}$ is not a completely arbitrary operator because it is constrained by some mathematical conditions. First, the energy functional $\tilde{E}$ has to be well defined. This is not a trivial property (in spite of the existing mapping $\tilde{\Psi} \rightarrow \rho$) because in the case of atomic nuclei the expectation value of the exact many-body Hamiltonian $H$ obtained with the quasiparticle-vacuum wave function can diverge due to the short-range singularity of the bare nucleon-nucleon ($NN$) forces. Thus, it is assumed that the effective Hamiltonian $\tilde{H}$ contains $NN$ forces whose matrix elements are well defined. Second, $\tilde{H}$ has to be chosen to ensure the minimal property of the total energy functional (see Eq. (26) below and Ref. [7] for more details). Using Eqs. (23) and (24) we can define, in analogy with Ref. [7], the residual correlation energy $E_{RC}$:

$$E_{RC}[\rho] = E[\rho] - \inf_{\tilde{\kappa}, \tilde{\kappa}^*} \tilde{E}[\rho, \tilde{\kappa}, \tilde{\kappa}^*] ,$$

(25)

and the total energy functional $E$:

$$E[\rho, \tilde{\kappa}, \tilde{\kappa}^*] = \tilde{E}[\rho, \tilde{\kappa}, \tilde{\kappa}^*] + E_{RC}[\rho] .$$

(26)

The main property of the total functional $E[\rho, \tilde{\kappa}, \tilde{\kappa}^*]$ is:

$$\inf_{\rho, \tilde{\kappa}, \tilde{\kappa}^*} E[\rho, \tilde{\kappa}, \tilde{\kappa}^*] = \inf_{\rho} \left( \inf_{\tilde{\kappa}, \tilde{\kappa}^*} \tilde{E}[\rho, \tilde{\kappa}, \tilde{\kappa}^*] + E_{RC}[\rho] \right) = \inf_{\rho} E[\rho] = E_{GS} ,$$

(27)

where $E_{GS}$ is the exact ground-state energy of the interacting system. If the infimum of the total functional (26) is the minimum (usual assumption which has to be fulfilled by an appropriate choice of the effective Hamiltonian $\tilde{H}$), it is attained for the true nonlocal ground-state DM $\rho$ as it follows from Eq. (23) and from the results of Sec. 2.

It is advisable to pass from the variables $\rho, \tilde{\kappa}$, and $\tilde{\kappa}^*$ in the functional $E$ to the components of the EDM $\mathcal{R}$ using Eqs. (13) for $\tilde{\kappa}$ and $\tilde{\kappa}^*$, and the relation

$$\rho(x,x') = \frac{1}{2} [ \delta(x',x) - \mathcal{R}(x',-;x,-) + \mathcal{R}(x,+;x',+) ]$$

(28)
which follows from Eqs. (13) at \( \tilde{\rho} = \rho \). Taking into account these relations, we introduce the energy functional \( E_{\text{ext}} \) depending on the EDM:

\[
E_{\text{ext}}[\mathcal{R}] = E[\rho, \tilde{\kappa}, \tilde{\kappa}^*].
\]  

(29)

It is obvious from Eqs. (27) and (29) that \( \inf_{\mathcal{R}} E_{\text{ext}}[\mathcal{R}] = E_{\text{GS}} \).

In order to establish the equations of motion of the theory, which will in the following be referred to as the Extended Density Matrix Functional Theory (EDMFT), let us define the functional

\[
F[\psi_{\lambda;+}, \psi_{\lambda;+}^*] = E_{\text{ext}}[\mathcal{R}] + \frac{1}{2} \sum_{\lambda, \chi} E_{\lambda} \int dx \left| \psi_{\lambda;+}(x; \chi) \right|^2 \\
- \frac{1}{2} \int dx \int dx' \mu(x, x') [\delta(x', x) + \sum_{\chi} \mathcal{R}(x', \chi; x, \chi)],
\]

(30)

where \( E_{\lambda} \) and \( \mu(x, x') = \mu_q \delta(x, x') \) are Lagrange multipliers introduced to ensure the normalization condition for \( \psi_{\lambda;+}(x; \chi) \) (see Eq. (3)) and the neutron and proton numbers conservation:

\[
\sum_{\sigma} \int d\mathbf{r} \rho(\mathbf{r}, \sigma, q; \mathbf{r}, \sigma, q) = N_q
\]

(31)

which are introduced through Eq. (28). Applying the variational principle to the functional \( F \), we obtain the following set of equations of motion (see Appendix A for details):

\[
\sum_{\chi'} \int dx' \mathcal{H}(x, \chi; x', \chi') \psi_{\lambda;\eta}(x'; \chi') = \eta E_{\lambda} \psi_{\lambda;\eta}(x; \chi),
\]

(32)

where

\[
\mathcal{H}(x, \chi; x', \chi') = 2 \frac{\delta E_{\text{ext}}[\mathcal{R}]}{\delta \mathcal{R}(x', \chi'; x, \chi)} - \chi \delta_{\chi, \chi'} \mu(x, x').
\]

(33)

These equations can also be written in the matrix form

\[
\begin{pmatrix}
    h - \mu & \Delta \\
    -\Delta^* & \mu - h^*
\end{pmatrix}
\begin{pmatrix}
    \psi_{\lambda;\eta}^{(+)} \\
    \psi_{\lambda;\eta}^{(-)}
\end{pmatrix}
= \eta E_{\lambda}
\begin{pmatrix}
    \psi_{\lambda;\eta}^{(+)} \\
    \psi_{\lambda;\eta}^{(-)}
\end{pmatrix},
\]

(34)

where \( h \) is the single-particle pseudo-Hamiltonian, \( \Delta \) is the operator of the pairing field:

\[
h(x, x') = \frac{\delta E[\rho, \tilde{\kappa}, \tilde{\kappa}^*]}{\delta \rho(x, x')}, \quad \Delta(x, x') = -2 \frac{\delta E[\rho, \tilde{\kappa}, \tilde{\kappa}^*]}{\delta \tilde{\kappa}^*(x', x)},
\]

(35)

and it is denoted: \( \psi_{\lambda;\eta}^{(\pm)} = \psi_{\lambda;\eta}(x; \pm) \). Obviously, we can consider \( E_{\lambda} > 0 \) (if \( E_{\lambda} < 0 \), the permutation \( \psi_{\lambda;+}(x; \chi) \leftrightarrow \psi_{\lambda;-}(x; \chi) \) is made). Thus, the Lagrange multipliers \( \mu_q \) and
$E_\lambda$ play the role of the chemical potential for the nucleons of the type $q$ and the role of
the absolute value of the quasiparticle energy respectively. From Eq. (34), the sense of the
indices $\eta$ and $\chi$, which appear in the functions $\psi_{\lambda,\eta}(x; \chi)$ introduced in Sec. 2 can be easily
understood. The index $\eta$ is the sign of the eigenvalue in Eq. (34), and $\chi$ denotes the upper
and the lower components of the eigenfunctions. In most cases one of these components is
small, and it completely vanishes for the blocked states in the CB representation (9) of the
functions $\psi_{\lambda,\eta}(x; \chi)$. However, in general, the functions of the CB representation, that is
$\tilde{\psi}_{\lambda,\eta}(x; \chi)$, are not solutions of Eq. (32), i.e. they are not eigenfunctions of the operator $\mathcal{H}$
(see comments in the Appendix B).

As it can be seen from Eq. (34), the equations of motion of the EDMFT have the
same form as the ones of the Hartree-Fock-Bogoliubov (HFB) theory. However, the EDMFT
is not reduced to this theory. First of all, the total energy functional (26) of the EDMFT
has a more general form as compared with the HFB energy functional. Actually, only the
part $\tilde{\mathcal{E}}$ corresponds to the HFB functional, whereas the term $E_{RC}$ has, in general, a more
complicated and less obvious functional dependence on the DM $\rho$. But the basic difference
between the HFB theory and the EDMFT is determined by the following: the EDMFT is
(in principle) an exact theory in the sense that Eqs. (27) are fulfilled. This is ensured by the
fact that the functional $E[\rho]$, which enters in the term $E_{RC}$, is defined by Eq. (23) through
a set of wave functions $\Psi$ which contains the exact wave function $\Psi_{GS}$ with a fixed
number of particles. In this sense one can say that in the EDMFT the number of particles is exactly
conserved, despite the auxiliary quantity $\tilde{\kappa}$, which has the sense of an anomalous DM (but
which does not coincide with $\kappa_{GS}$), takes nonzero values. In this context, the HFB theory can
be considered as the phenomenological realization of the EDMFT. The relationship between
EDMFT and HFB approaches is analogous to the relationship between the theory developed
in Ref. [7] and the density-dependent Hartree-Fock theory, as it was discussed in more detail
in Ref. [7].

4 REDUCTION TO THE EXTENDED QUASILOCAL THEORY

The theory developed in the previous sections is essentially a nonlocal one as can be seen from
Eqs. (34) and (35). The exact solution of that equations is a rather complicated problem.
However, one can noticeably simplify the task of solving these equations by reducing the
total energy functional $\mathcal{E}[\rho, \tilde{\kappa}, \tilde{\kappa}^*]$ to a quasilocal form following the method described in
Ref. [7].

In the particular case of atomic nucleus let us introduce a set of local quantities consisting of the local particle $n_q$, the kinetic-energy $\tau_q$, and the spin $J_q$ densities for neutrons and protons which are obtained from the nonlocal DM $\rho$ as:

$$n_q(r) = \sum_\sigma \int dx' \delta(x,x') \rho(x,x'), \quad (36)$$
$$\tau_q(r) = \sum_\sigma \int dx' \delta(x,x') (\nabla_r \nabla_{r'}) \rho(x,x'), \quad (37)$$
$$J_q(r) = i \sum_\sigma \int dx' \delta(r - r') \delta_{q,q'} [\sigma \delta \times \nabla_r] \rho(x,x'). \quad (38)$$

Note that in contrast to the analogous definitions of Ref. [7], in this case the exact DM $\rho$ enters in Eqs. (36) – (38) (see remark after Eq. (27)), so the quantities $\tau_q$ and $J_q$ are the exact (correlated) neutron and proton kinetic-energy and spin densities respectively.

Explicit expressions for these local quantities, which follow from Eqs. (16) and from the representation of the EDM in the form (10), are:

$$n_q(r) = \sum_\sigma \sum_\lambda |\psi_{\lambda^{-}}(r,\sigma,q;+)|^2, \quad (39)$$
$$\tau_q(r) = \sum_\sigma \sum_\lambda |\nabla \psi_{\lambda^{-}}(r,\sigma,q;+)|^2, \quad (40)$$
$$J_q(r) = i \sum_\sigma \sum_\sigma' \sum_\lambda \psi_{\lambda^{-} \sigma'}^* (r,\sigma',q;+) [\sigma \delta \times \nabla] \psi_{\lambda^{-}} (r,\sigma,q;+). \quad (41)$$

We can also define the quantities $\kappa_q$ which have the meaning of local anomalous densities for each kind of nucleons as:

$$\kappa_q(r) = i \sum_\sigma \int dx' \delta(r - r') \delta_{q,q'} (\sigma_y) \sigma' \kappa(x,x') \quad (42)$$
$$= i \sum_\sigma \sum_\lambda \psi_{\lambda^{-} \sigma'}^* (r,\sigma,q;+) [\sigma \delta \times \nabla] \psi_{\lambda^{-}} (r,\sigma,q;+). \quad (43)$$

Let us now introduce three kinds of the short notations: $\rho_{QL} = \{n_n, n_p, \tau_n, \tau_p, J_n, J_p\}$, $\kappa = \{\kappa_n, \kappa_p\}$, and $\kappa^* = \{\kappa_n^*, \kappa_p^*\}$. Using these notations, we define the following quasilocal energy functionals:

$$\mathcal{E}_{QL1}[\rho_{QL}, \kappa, \kappa^*] = \inf_{\rho \to \rho_{QL}} \mathcal{E}[^{\rho} \to \rho_{QL} \kappa, \kappa^*], \quad (44)$$
$$\mathcal{E}_{QL2}[\rho_{QL}, \kappa, \kappa^*] = \inf_{\rho \to \rho_{QL}} \inf_{\kappa \to \kappa^*} \inf_{\kappa^* \to \kappa^*} \mathcal{E}[^{\rho} \to \rho_{QL} \kappa, \kappa^*]. \quad (45)$$
Note that the mappings $\rho \rightarrow \rho^{QL}$, $\tilde{\kappa} \rightarrow \kappa$, and $\tilde{\kappa}^* \rightarrow \kappa^*$ are established according to Eqs. (36) – (38) and (42). From the definitions (44) – (45), it immediately follows that the property (27) is also true for both energy functionals $E^{QL1}$ and $E^{QL2}$. Namely, we have

$$\inf_{\rho^{QL}, \kappa, \kappa^*} E^{QL1}[\rho^{QL}, \tilde{\kappa}, \tilde{\kappa}^*] = \inf_{\rho^{QL}, \kappa, \kappa^*} E^{QL2}[\rho^{QL}, \kappa, \kappa^*] = E_{GS}.$$ (46)

In the following we shall refer to the theories based on the functionals (44) and (45) as the extended quasilocal density functional theories EQLT1 and EQLT2.

The equations of motion for these quasilocal theories have the same matrix form (34), as for the nonlocal theory, but with different definitions of the operators $h$ and $\Delta$. Making use of Eqs. (35) and (36) – (38), we obtain

$$h(x, x') = \delta_{q, q'} \left\{ -\nabla_r \frac{\hbar^2}{2m_q^*(r)} \nabla_r + U_q(r) \right\} \delta_{\sigma, \sigma'} - i W_q(r) \cdot [\nabla_r \times \sigma]_{\sigma, \sigma'} \delta(r - r'),$$ (47)

where for the quasilocal theory EQLT1:

$$\frac{\hbar^2}{2m_q^*(r)} = \frac{\delta E^{QL1}}{\delta \tau_q(r)}, \quad U_q(r) = \frac{\delta E^{QL1}}{\delta n_q(r)}, \quad W_q(r) = \frac{\delta E^{QL1}}{\delta J_q(r)},$$ (48)

and analogous expressions with the replacement of $E^{QL1}$ by $E^{QL2}$ in the case of the quasilocal theory EQLT2. The difference between these two versions of the quasilocal approach consists in the definition of the operator $\Delta$. Within the EQLT1 we have

$$\Delta(x, x') = -2 \frac{\delta E^{QL1}}{\delta \tilde{\kappa}^*(x', x)},$$ (49)

as in the nonlocal theory, whereas in the case of the EQLT2 the operator $\Delta$ is purely local and it is obtained using Eq. (42)

$$\Delta(x, x') = -2 i \delta(r - r') \delta_{q, q'} (\sigma_y)_{\sigma, \sigma'} \frac{\delta E^{QL2}}{\delta \kappa^*_q(r)}.$$ (50)

Let us stress that the solution of the equations of motion associated with both EQLT1 and EQLT2 enables us (at least in principle) to calculate the exact values of all the local densities entering in the set $\rho^{QL}$. The theory of Ref. [7] allows to find the exact values of the local particle densities $n_q(r)$ only. This difference comes from different character of the many-fermion wave functions used for the building of the energy functional: a Slater-determinant wave function in [7] for which only the Lieb theorem was proved, and a quasiparticle-vacuum wave function in the present paper which enables one, as it was shown, to reproduce an arbitrary nonlocal DM $\rho$. 

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Comparing our approach with theory developed in Ref. [3], it should be noted that we do not introduce any external anomalous pair potential as it was done in [3]. In our method the pairing emerges only as a consequence of the interaction between the fermions. In absence of the interaction the pairing field $\Delta$ vanishes, which is in agreement with the particle-number conservation condition. The same difference exists between the equations of motion of the EQLT2 case and the Bogoliubov-de Gennes equations [12] in which the pair potential enters, in fact, as an external field (though created initially by the interaction).

It should also be pointed out that the EDMFT in its nonlocal and quasilocal versions can be reduced to the more simple DFT plus BCS description of the pairing correlations if the operator $H$ in Eq. (32) is (or is assumed to be) diagonal in the CB representation [9]. However, in general, this description is not equivalent to the one obtained by solving exactly the EDMFT equations of motion (see comments in the Appendix B). This reduction of the EDMFT is analogous to the replacement of the HFB equations by coupled Hartree-Fock plus BCS equations how it is discussed in Refs. [8, 9].

5 SUMMARY AND CONCLUSIONS

We have extended the recently developed quasilocal density functional theory [7] to include pairing correlations. This new approach named Extended Density Matrix Functional Theory is based on an extended density matrix (EDM) formalism. The EDM $R$ contains as a block the normal density matrix $\rho$ and as another block an auxiliary quantity $\tilde{\kappa}$ which has the sense of an anomalous density matrix, but which does not coincide with the exact one $\kappa$ in general. The matrix $\tilde{\kappa}$ is chosen in such a way that the equality $R^2 = R$ is fulfilled. The EDM which possesses this property can be easily constructed for a given density matrix $\rho$ using the canonical basis in which $\rho$ is diagonal. It has been shown that for an arbitrary density matrix $\rho$, corresponding to some interacting time-reversal invariant fermion system, there exist a quasiparticle-vacuum wave function $\tilde{\Psi}$ and an EDM $R$ such that the following many-to-one mappings take place: $\tilde{\Psi} \rightarrow R \rightarrow \rho$. This statement can be considered as a generalization of the Lieb theorem. Using the connection between $R$ and $\rho$, we have defined the total energy functional as an extended functional of $R$. It has been proved that its minimum value is equal to the exact ground state energy of the considered system. This extended energy functional is reduced further to a quasilocal form. Thus, in the corresponding final equations of motion the single-particle pseudo-Hamiltonian $h$ and the pairing field $\Delta$ are
both (quasi) local. Although the equations of motion in our theory have the same form as 
the ones of the Hartree-Fock-Bogoliubov theory, the main difference is that the Extended 
Density Matrix Functional Theory is, in principle, an exact theory in the sense that the true 
ground stated energy can be reached for the true normal density matrix $\rho$. Finally, notice 
that the general formalism developed in this work, which introduces the pairing correlations 
in the DFT, has been discussed in the particular case of the atomic nucleus, but it can be 
easily applied to other Fermi systems with a fixed number of particles.

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APPENDIX A

In this Appendix the equations of motion of the EDMFT are derived. Varying the functional 
$F$ defined by Eq. (30) and taking into account Eq. (10), we obtain:

$$
\delta F = \sum_{\lambda,\chi,\chi'} \int dx \, dx' \left\{ \frac{\delta E_{\text{ext}}[\mathcal{R}]}{\delta \mathcal{R}(x', \chi'; x, \chi)} - \frac{1}{2} \delta_{\chi,\chi'} [\chi \mu(x, x') - \delta(x, x') E_{\lambda}] \right\} \times \left[ \psi_{\lambda,-}(x'; \chi') \delta \psi_{\lambda,-}^*(x; \chi) + \psi_{\lambda,-}^*(x; \chi) \delta \psi_{\lambda,-}(x'; \chi') \right] = 0. 
$$

(A1)

This leads to the following equations of motion:

$$
\sum_{\chi'} \int dx' \, \mathcal{H}(x, \chi; x', \chi') \psi_{\lambda,-}(x'; \chi') = -E_{\lambda} \psi_{\lambda,-}(x; \chi),
$$

(A2)

where the operator $\mathcal{H}$ is defined by Eq. (33). The Eq. (A2) formally defines only one half 
of the complete set of the eigenfunctions of $\mathcal{H}$. In order to define second half, let us note first 
that if the following equalities are fulfilled

$$
\mathcal{H}(x, \chi; x', \chi') = -\mathcal{H}(x', -\chi'; x, -\chi) = \mathcal{H}^*(x', \chi'; x, \chi),
$$

(A3)
then the functions $\psi_{\lambda;+}(x; \chi)$, defined through the functions $\psi_{\lambda;-}(x; \chi)$ using the condition (7), are also the eigenfunctions of $\mathcal{H}$. In this case the complete set of the eigenfunctions of $\mathcal{H}$ is divided into two equal parts with eigenvalues $+E_\lambda$ and $-E_\lambda$. On the other hand, if the condition (7) is fulfilled, and if the set of the functions $\psi_{\lambda;-}(x; \chi)$ is taken as a half of the complete set $\{\psi_{\lambda;\pm}(x; \chi)\}$, then Eq. (12) is true, and it follows from Eq. (33) that Eqs. (A3) are also fulfilled. Consequently, properties (7) and (A3) follow from each other, and there exists a solution of the equations of motion which possesses both properties. So, setting Eq. (7) to be satisfied, we actually choose a solution which has the symmetry defined by this equation without imposing additional constraints in the variational procedure. In that case, using Eqs. (7) and (A3), we come from (A2) to Eq. (32) which represents complete set of the equations of motion.

**APPENDIX B**

In this Appendix the relationship between the eigenfunctions of the operators $\mathcal{R}$ and $\mathcal{H}$ is analyzed. First of all, notice that from Eqs. (10) and (5) it follows that

$$\sum_{\chi'} \int dx' \mathcal{R}(x, \chi; x', \chi') \psi_{\lambda;\eta}(x'; \chi') = \delta_{\eta,-} \psi_{\lambda;\eta}(x; \chi).$$

(B1)

Thus, the functions $\psi_{\lambda;\eta}(x; \chi)$ are eigenfunctions of the operator $\mathcal{R}$. Obviously, the set of the eigenfunctions of $\mathcal{R}$ is determined by a given $\mathcal{R}$ up to an arbitrary unitary transformation of the type Eq. (8). Consequently, the functions $\tilde{\psi}_{\lambda;\eta}(x; \chi)$ defined by Eqs. (9) are also eigenfunctions of the operator $\mathcal{R}$. On the other hand, from Eqs. (B1) and (32) it follows that there exists at least one set of eigenfunctions (namely the set $\{\psi_{\lambda;\eta}(x; \chi)\}$) which is common for both operators $\mathcal{R}$ and $\mathcal{H}$. However, from these equations it does not follow that any eigenfunction of $\mathcal{R}$, and in particular $\tilde{\psi}_{\lambda;\eta}(x; \chi)$, will be also eigenfunction of $\mathcal{H}$. Indeed, while a set of eigenfunctions of $\mathcal{R}$ is determined up to an arbitrary unitary transformation (8), this is not true for the eigenfunctions of $\mathcal{H}$, since Eqs. (32) and (34) are not covariant under this transformation. Consequently, if we use an arbitrarily given representation of the eigenfunctions of the operator $\mathcal{R}$, in particular the CB representation (9), an additional nontrivial $C$-transformation, which does not change $\mathcal{R}$, is generally required to diagonalize $\mathcal{H}$ (see Refs. [8, 9] for details).
References

[1] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).

[2] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133 (1965).

[3] L. N. Oliveira, E. K. U. Gross, and W. Kohn, Phys. Rev. Lett. 60, 2430 (1988).

[4] S. A. Fayans, S. V. Tolokonnikov, E. L. Trykov, and D. Zawischa, Nucl. Phys. A 676, 49 (2000).

[5] A. Bulgac, Phys. Rev. C 65, 051305(R) (2002).

[6] T. L. Gilbert, Phys. Rev. B 12, 2111 (1975).

[7] V. B. Soubbotin, V. I. Tselyaev, and X. Viñas, Phys. Rev. C 67, 014324 (2003).

[8] P. Ring and P. Schuck, The Nuclear Many-Body Problem (Springer-Verlag, New York Inc., 1980).

[9] J. Dobaczewski, W. Nazarewicz, T. R. Werner, J. F. Berger, C. R. Chinn, and J. Dechargé, Phys. Rev. C 53, 2809 (1996).

[10] C. Bloch and A. Messiah, Nucl. Phys. 39, 95 (1962).

[11] E. H. Lieb, Int. J. Quantum Chem. 24, 243 (1983).

[12] P. G. de Gennes, Superconductivity of Metals and Alloys (Benjamin, New York, 1966).