Generalization of Lieb’s variational principle to Bogoliubov–Hartree–Fock theory

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In its original formulation, Lieb’s variational principle holds for fermion systems with purely repulsive pair interactions. As a generalization we prove for both fermion and boson systems with semi-bounded Hamiltonian that the infimum of the energy over quasifree states coincides with the infimum over pure quasifree states. In particular, the Hamiltonian is not assumed to preserve the number of particles. To shed light on the relation between our result and the usual formulation of Lieb’s variational principle in terms of one-particle density matrices, we also include a characterization of pure quasifree states by means of their generalized one-particle density matrices. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4853875]

I. INTRODUCTION

The Rayleigh–Ritz variational principle for the ground state energy is the starting point of many computations and approximations in quantum chemistry. For a many-particle system whose dynamics is generated by a Hamiltonian $H$, it can be written as

$$E_{gs} = \inf \left\{ \text{tr}_{F^\pm}(\rho H) \mid \rho \geq 0, \text{tr}_{F^\pm}(\rho) = 1 \right\},$$

where $\rho$ varies over the density matrices on the Fock space $F^\pm \equiv F^\pm[\hbar]$ of the system ($E_{gs}$ in (1) is actually the total ground state energy in the grand canonical ensemble). A typical many-particle Hamiltonian is given as the sum $H = h + V$ of the second quantization $h$ of a one-particle operator $h$ and the second quantization $V$ of a pair potential $V$. Since $h$ is quadratic and $V$ is quartic in the field operators, one can rewrite (1) in terms of the one-particle density matrix (1-pdm) $\gamma_\rho \in L^1(h)$ and the two-particle density matrix (2-pdm) $\Gamma_\rho \in L^1(h \otimes h)$ of a given density matrix $\rho \in L^1(F^\pm)$ as

$$E_{gs} = \inf \left\{ \mathcal{E}(\gamma_\rho, \Gamma_\rho) \mid \rho \geq 0, \text{tr}_{F^\pm}(\rho) = 1 \right\},$$

where the energy functional $\mathcal{E}$ is defined by

$$\mathcal{E}(\gamma_\rho, \Gamma_\rho) := \text{tr}_h(h \gamma_\rho) + \frac{1}{2} \text{tr}_h(V \Gamma_\rho).$$

The computation of the ground state energy and the corresponding ground state vector of a quantum mechanical many-particle system is a complex, if not impossible, task and one resorts to approximation methods. The Hartree–Fock approximation is one of the first approximations that emerged from
ground state computations in quantum chemistry\textsuperscript{2,4,5} In its original formulation, the Rayleigh–Ritz principle for the ground state energy in terms of wave functions,

\[ E_{gs} = \inf \left\{ \langle \Psi, \hat{H} \Psi \rangle \mid \Psi \in \mathcal{F}^-, \| \Psi \|_{\mathcal{F}^-} = 1 \right\}, \]

of a fermion system with Hamiltonian \( \hat{H} \) is replaced by a variation over Slater determinants,

\[ E_{\text{HF}} = \inf \left\{ \langle \Phi, \hat{H} \Phi \rangle \mid N \in \mathbb{N}, \Phi = \varphi_1 \wedge \ldots \wedge \varphi_N, \langle \varphi_i, \varphi_j \rangle_{\mathbb{H}} = \delta_{i,j} \right\}, \tag{2} \]

where the Hamiltonian \( \hat{H} \) conserves the particle number, i.e., \( [\hat{H}, \mathbb{N}] = 0 \), with \( \mathbb{N} \) being the particle number operator. The density matrix \( \rho = |\Phi\rangle \langle \Phi| \) associated to a Slater determinant is a pure, particle number-conserving, quasifree density matrix and (2) can be rewritten as

\[ E_{\text{HF}} = \inf \left\{ \text{tr}_{\mathcal{F}^-}(\rho \mathbb{H}) \mid \rho \text{ is a pure, particle number-conserving, quasifree density matrix} \right\}. \]

Since the one-particle density matrix \( \gamma \) of a fermion Slater determinant \( \Phi = \varphi_1 \wedge \ldots \wedge \varphi_N \) is the range-N orthogonal projection onto \( \text{span}\{\varphi_1, \ldots, \varphi_N\} \) and its two-particle density matrix is given as \( \Gamma = (\mathbb{1}_{\mathbb{H}\mathbb{H}} - \text{Ex})\gamma \otimes \gamma \), the Hartree–Fock energy can be written as

\[ E_{\text{HF}} = \inf \left\{ \mathcal{E}(\gamma, (\mathbb{1}_{\mathbb{H}\mathbb{H}} - \text{Ex})\gamma) \mid \gamma = \gamma^*, \text{tr}_{\mathbb{H}}(\gamma) < \infty \right\}. \]

In case of purely repulsive pair potentials \( V \), Lieb’s variational principle\textsuperscript{2,5,14} asserts that

\[ E_{\text{HF}} = \inf \left\{ \mathcal{E}(\gamma, (\mathbb{1}_{\mathbb{H}\mathbb{H}} - \text{Ex})\gamma) \mid 0 \leq \gamma \leq \mathbb{1}_{\mathbb{H}}, \text{tr}_{\mathbb{H}}(\gamma) = N \right\}. \]

Going back to a description on the Fock space, Lieb’s variational principle reads

\[ E_{\text{HF}} = \inf \left\{ \text{tr}_{\mathcal{F}^-}(\rho \mathbb{H}) \mid \rho \text{ is a particle number-conserving, quasifree density matrix} \right\}, \tag{3} \]

i.e., it asserts that the pureness requirement of the quasifree density matrix can be dropped. As was shown in Ref. 5, the property \( [\rho, \mathbb{N}] = 0 \) of particle number conservation is also obsolete for repulsive pair potentials \( V \), and the Hartree–Fock energy \( E_{\text{HF}} \) agrees with the Bogoliubov–Hartree–Fock (BHF) energy \( E_{\text{BHF}} \) defined by

\[ E_{\text{BHF}} := \inf \left\{ \text{tr}_{\mathcal{F}^-}(\rho \mathbb{H}) \mid \rho \text{ is a quasifree density matrix} \right\}. \tag{4} \]

Our main result is a generalization of Lieb’s variational principle (3) in several ways. Namely, we show that the infimum in (4) is already obtained from a variation over pure quasifree density matrices,

\[ E_{\text{BHF}} = E_{\text{BHF}}^{\text{pure}} := \inf \left\{ \text{tr}_{\mathcal{F}^\pm}(\rho \mathbb{H}) \mid \rho \text{ is a pure quasifree density matrix} \right\}. \]

under the mere assumption that \( \mathbb{H} \) is bounded below. Neither repulsiveness of the pair potential \( V \) nor the form \( \mathbb{H} = \mathbb{h} + V \) or even the conservation of the particle number by \( \mathbb{H} \) is assumed. Furthermore, we show that \( E_{\text{BHF}} = E_{\text{BHF}}^{\text{pure}} \) for both fermion and boson systems. The precise formulation of this result and its proof is given in Theorem 3.1. Note that, especially for boson systems, it is crucial that our result does not require the Hamiltonian to conserve the particle number because for most physically interesting models such an assumption would not be fulfilled.

The above result, i.e., Theorem 3.1, brings pure quasifree density matrices \( \rho \) into focus. These are fully characterized by their generalized one-particle density matrix \( \gamma_\rho \) defined in terms of their two-point correlation functions as

\[ \left\{ f_1 \oplus f_2, \gamma_\rho(g_1 \oplus g_2) \right\}_{\mathbb{h} \mathbb{h}} := \text{tr}_{\mathcal{F}^\pm} \left( \rho \left[ a^*(g_1) + a(g_2) \right] \left[ a(f_1) + a^*(f_2) \right] \right), \]

where \( \{a^*(f), a(f) \mid f \in \mathbb{h}\} \) are the usual boson or fermion creation operators on \( \mathcal{F}^\pm \) fulfilling the canonical commutation or anticommutation relations, respectively, with \( a(f) \) annihilating the vacuum and \( f \mapsto J(f) := \overline{f} \) being a fixed antilinear involution on \( \mathbb{h} \) which we refer to as the complex conjugation. Here, we implicitly assume \( \text{tr}_{\mathcal{F}^\pm}(\rho a(f)) = 0 \), for all \( f \in \mathbb{h} \), i.e., \( \rho \) is \textit{centered}. This assumption is irrelevant for fermion systems and made without loss of generality for boson systems,
as is explained below. The higher correlation of the (centered) quasifree density matrix \( \rho \) can be computed from sums over products of the two-point correlation function, i.e., in terms of \( \tilde{\gamma}_\rho \), using Wick’s Theorem. It is well-known\(^5\),\(^7\) that, as a 2 \( \times \) 2 matrix with operator-valued entries, \( \tilde{\gamma}_\rho \) can be written as

\[
\tilde{\gamma}_\rho = \begin{pmatrix}
\gamma_\rho & \alpha_\rho \\
\overline{\alpha}_\rho & \mathbb{1}_\mathbb{B} \pm \overline{\gamma}_\rho
\end{pmatrix}, \quad \gamma_\rho = \gamma^*_\rho, \quad \alpha_\rho = \pm \alpha^*_\rho,
\]

where \(+\) holds for boson and \(-\) for fermion systems, and \( \overline{A} := JAJ \) denotes the complex conjugate and \( A^T := \overline{A}^* \) the transpose of a bounded operator \( A \in \mathcal{B}(\mathbb{H}) \). It is easy to check that

\[
0 \leq \tilde{\gamma}_\rho \leq 1_{\mathbb{B} \otimes \mathbb{B}}, \quad \text{for fermion systems},
\]

\[
\tilde{\gamma}_\rho = 1_{\mathbb{B} \otimes \mathbb{B}}, \quad \text{for boson systems},
\]

\[
\tilde{\gamma}_\rho = \overline{\gamma}_\rho, \quad \text{for fermion systems},
\]

\[
\tilde{\gamma}_\rho = -\gamma_\rho S \overline{\gamma}_\rho, \quad \text{for boson systems},
\]

We restrict our attention to density matrices with finite particle number expectation, for which \( \text{tr}_\mathbb{B}(\gamma_\rho) = \text{tr}_{\mathbb{F}^\pm}(\rho \mathbb{N} \mathbb{N}) < \infty \). In this case, it is well-known that the converse of (6) and (7) holds true in the sense that, given \( \tilde{\gamma} \) as in (5), with \( \gamma = \gamma^* \in \mathcal{L}(\mathbb{H}) \), \( \gamma \geq 0 \), \( \alpha = \pm \alpha^* \), and obeying \( \gamma \geq 0 \) for bosons systems, or \( 0 \leq \tilde{\gamma} \leq 1_{\mathbb{B} \otimes \mathbb{B}} \) for fermions systems, there exists a centered quasifree density matrix \( \rho \in \mathcal{L}_1(\mathcal{F}) \) such that \( \tilde{\gamma} = \gamma_\rho \).

It is furthermore well-known\(^5\),\(^7\) that, if \( \rho \) is a pure quasifree density matrix, then

\[
\tilde{\gamma}_\rho = \gamma_\rho^2, \quad \tilde{\gamma}_\rho = \gamma_\rho^2, \quad \text{for fermion systems, and}
\]

\[
\tilde{\gamma}_\rho = -\gamma_\rho S \overline{\gamma}_\rho, \quad \text{for boson systems},
\]

where \( \mathcal{S} = \mathbb{1}_\mathbb{B} \oplus (-\mathbb{1}_\mathbb{B}) \). We show that also the converse statement holds true: If the generalized one-particle density matrix \( \tilde{\gamma}_\rho \) of a density matrix \( \rho \) fulfills (8) in the fermion case or (9) in the boson case, then the density matrix is pure and quasifree. Note that the quasifreeness of \( \rho \) is asserted, not assumed. The precise formulation of this result is given in Theorem 4.1.

In the Appendix, we derive representability conditions on the two-particle density matrix \( \Gamma_\rho \) of a boson density matrix \( \rho \). Similar to \( \Gamma_\mathcal{G} \), \( \Gamma_\mathcal{P} \), and \( \Gamma_\mathcal{Q} \)-conditions for fermion reduced density matrices, these conditions follow from the positivity

\[
\text{tr}_{\mathbb{F}^\pm}(\rho P_2^\ast(a^*, a) P_2(a^*, a)) \geq 0
\]

(10)

of the density matrix \( \rho \) on positive observables of the form \( P_2^\ast(a^*, a) P_2(a^*, a) \), where \( P_2(a^*, a) \) is a polynomial of degree 2 or smaller in the creation and annihilation operators. A crucial difference, however, is that \( \rho \) is not assumed to be particle number-conserving, as this would not be a fair assumption for boson systems. Hence, the reduction of the general condition (10) to simpler conditions like \( \Gamma_\mathcal{G} \), \( \Gamma_\mathcal{P} \), and \( \Gamma_\mathcal{Q} \) is not as straightforward as in the fermion case and is, in fact, not carried out in this paper, but is subject to future work.

II. SECOND QUANTIZATION AND BOGOLIUBOV–HARTREE–FOCK THEORY

A. Second quantization

We first introduce our notations concerning the objects used in the method of second quantization. More information can be found in Refs. 6–9, 18, and 19.

Let \( (\mathbb{H}, \langle . , . \rangle_\mathbb{H}) \) be a complex separable Hilbert space, to which we refer as the one-particle Hilbert space. We consider both the case of bosons and fermions. When they are different, the sign above denotes the case of bosons and the sign below the case of fermions. The boson, resp. fermion Fock space \( \mathcal{F}^\pm \) is the direct sum of all symmetric, resp. antisymmetric \( N \)-particle Hilbert spaces: \( \mathcal{F}^\pm \equiv \mathcal{F}^\pm[\mathbb{H}] := \bigoplus_{N=0}^{\infty} \mathcal{S}_N^\pm \mathbb{H} \otimes \mathbb{H}^\otimes N \). Here, by convention \( \mathbb{H}^\otimes 0 := C \) and the symmetrization, resp. antisymmetrization operator \( \mathcal{S}_N^+ \) is the linear operator on \( \mathbb{H} \otimes \mathbb{H}^\otimes N \) such that

\[
\mathcal{S}_N^+ \left( f^{(N)} \right) = \frac{1}{N!} \sum_{\pi \in \Theta_N} (\pm 1)^\pi \bigotimes_{k=1}^{N} f_{\pi(k)}^{(N)}
\]
for $f^{(N)} = \bigotimes_{k=1}^{N} f_{k}^{(N)} \in \mathfrak{h}^{\otimes N}$, where $\mathfrak{S}_N$ denotes the symmetric group and $(\pm 1)^v$ denotes 1, resp. the signature of the permutation $\pi$. The Fock space $\mathcal{F}^\pm$ equipped with the inner product $\langle \Psi_j, \Psi_j \rangle_{\mathcal{F}^\pm} := \sum_{N=0}^{\infty} \langle f^{(N)}_j, \psi^{(N)}_j \rangle_{\mathcal{H}^\otimes N}$ for any $\Psi_j := \langle f^{(N)}_j \rangle_{N=0}$ is a Hilbert space. The vacuum vector is the sequence $\Omega := (1, 0, 0, \ldots) \in \mathcal{F}^\pm$.

The particle number operator is defined as $\hat{N} := \bigoplus_{N=0}^{\infty} N 1_{\mathcal{H}^\otimes N}$ and, for any bounded operator $B \in \mathcal{B}(\mathfrak{h})$, $\Gamma(B) := \bigoplus_{N=0}^{\infty} B^\otimes N$ is an operator on $\mathcal{F}^\pm$. In particular, $\Gamma(B)$ is trace class ($\Gamma(B) \in \mathcal{L}^1(\mathcal{F})$), if $B \in \mathcal{L}^1(\mathfrak{h})$ and, for bosons, additionally $\|B\|_{\mathcal{B}(\mathfrak{h})} \leq 1$.

For any $f \in \mathfrak{h}$, the boson creation and annihilation operators are denoted by $a^*(f)$ and $a(f)$, respectively. They are completely characterized by the properties $a(f) \Omega = 0$, $a^*(f) \Omega = f$, and, in the case of bosons, the canonical commutation relations (CCR)

$$\{a^*(f), a(g)\} = 0 = [a(f), a(g)] \quad \text{and} \quad [a(f), a^*(g)] = (f, g)_{\mathfrak{h}} 1_{\mathcal{F}^+},$$

for any $f, g \in \mathfrak{h}$, where $[A, B] := AB - BA$ is the commutator, or in the case of fermions, the canonical anticommutation relations (CAR)

$$\{a^*(f), a(g)\} = 0 = [a(f), a(g)] \quad \text{and} \quad \{a(f), a^*(g)\} = (f, g)_{\mathfrak{h}} 1_{\mathcal{F}^-},$$

for any $f, g \in \mathfrak{h}$, with the anticommutator $\{A, B\} := AB + BA$. We use the abbreviations $a^*_k = a^* (\phi_k)$ and $a_k = a (\phi_k)$ for a fixed, but arbitrary orthonormal basis (ONB) $\{\phi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$.

In the case of bosons, we additionally need Weyl operators and Weyl transformations. For every $f \in \mathfrak{h}$, the unitary transformation $\mathbb{W}(f) : \mathcal{F}^{\pm} \to \mathcal{F}^{\pm}$, called Weyl operator, is defined by $\mathbb{W}(f) := \exp(i\Phi(f))$, where $\Phi(f) := (a^*(f) + a(f)) / \sqrt{2}$. The Weyl operators satisfy $\mathbb{W}(f)^* = \mathbb{W}(-f)$ and the Weyl commutation relations

$$\mathbb{W}(f) \mathbb{W}(g) = e^{-i \text{Im}(f, g)_{\mathfrak{h}}} \mathbb{W}(f + g)$$

for any $f, g \in \mathfrak{h}$. $\mathbb{W}_F \equiv \mathbb{W}(i\sqrt{2}g)$ defines a unitary transformation, called Weyl transformation, for any $g \in \mathfrak{h}$. For any $f \in \mathfrak{h}$, this transformation yields

$$\mathbb{W}_F a^*(f) \mathbb{W}_F^* = a^*(f) + (g, f)_{\mathfrak{h}} \quad \text{and} \quad \mathbb{W}_F a(f) \mathbb{W}_F^* = a(f) + (f, g)_{\mathfrak{h}}.$$

### 1. Bogoliubov transformation

In this section, we fix an (arbitrary) orthonormal basis $\{\phi_k\}_{k=1}^{\infty}$ of $\mathfrak{h}$. As the definitions of complex conjugates of both a wave function and an operator depend on the choice of the ONB of $\mathfrak{h}$, so do the transforms defined in the following. We refer the reader to Refs. $15$ and $18$ for a basis independent formulation.

Let $\{\phi_k\}_{k=1}^{\infty}$ be an ONB of $\mathfrak{h}$. The complex conjugate of a function $f = \sum_{k=1}^{\infty} \mu_k \phi_k \in \mathfrak{h}$, with $(\mu_k) \in \ell^2(\mathbb{N})$, is defined by

$$\overline{f} := \sum_{k=1}^{\infty} \overline{\mu_k} \phi_k.$$

Furthermore, we define for any operator $A$ the complex conjugate operator $\overline{A}$ by

$$\langle f, \overline{A} g \rangle := \langle \overline{f}, A \overline{g} \rangle.$$

For any linear operator $A$, the transpose is defined as $A^T := \overline{A} = \overline{A^T}$. Now, we are prepared to define a Bogoliubov transformation.

**Definition 2.1**. A linear map $U = \left( \begin{array}{cc} u & v \\ \overline{v} & \overline{u} \end{array} \right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ is called boson, resp. fermion Bogoliubov transformation if the linear operators $u : \mathfrak{h} \to \mathfrak{h}$ and $v : \mathfrak{h} \to \mathfrak{h}$ fulfill in the case of bosons

\[ u^* u - u u^* = 1_{\mathfrak{h}}, \quad u^* u - u u^* = 1_{\mathfrak{h}} \]  

(1a)  

\[ u^* v - v^* u = 0, \quad u v^* - v u^* = 0, \]  

(1b)
and in the case of fermions
\[ uu^* + vv^* = 1, \quad u^*u + v^*v = 1, \tag{12a} \]
\[ u^*v + v^*u = 0, \quad uv^* + vu = 0. \tag{12b} \]

Remark 2.2. Any Bogoliubov transformation \( U \) is invertible. In the case of bosons, Eqs. (11a) and (11b) on \( u \) and \( v \) are equivalent to stating \( U^*SU = S, U^*S = S \) with \( S := \mathbb{1}_\mathbb{h} \otimes (-\mathbb{1}_\mathbb{h}) \). The inverse of \( U \) is thus given by the boson Bogoliubov transformation \( U^{-1} = SU^* \). In the case of fermions, Eqs. (12a) and (12b) on \( u \) and \( v \) are equivalent to the condition that \( U \) is unitary. Therefore, the inverse of a fermion Bogoliubov transformation \( U \) is the Bogoliubov transformation \( U^* \).

Lemma 2.3. Let \( U = \left(\begin{array}{cc} u & v \\ \pi & \pi \end{array}\right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h} \) be a boson, resp. fermion Bogoliubov transformation. There is a unitary transformation \( U_U : \mathcal{F}^\pm \to \mathcal{F}^\pm \) such that
\[ U_U \left[ a^*(f) + a(\overline{g}) \right] U_U^* = a^*(uf + vg) + a(vf^* + u\overline{g}) \]
for all \( f, g \in \mathfrak{h} \) if and only if \( v \) is Hilbert–Schmidt. We call \( U_U \) unitary representation or implementation of \( U \) on \( \mathcal{F}^\pm \).

The Hilbert–Schmidt condition on \( v \) is called Shale-Stinespring condition. The proof of this lemma (in the case of fermions) can be found, for instance, in Ref. 1.

2. States and quasi-free states

We consider states \( \omega \) as being continuous, linear forms on the CCR algebra \( \mathcal{A}^+ \) generated by Weyl operators in the case of bosons or on the CAR algebra \( \mathcal{A}^- \) generated by the identity, creation, and annihilation operators in the case of fermions such that \( \omega \) is positive and \( \omega(1_{\mathcal{F}^\pm}) = 1 \). In fact, we restrict our attention to normal states (with respect to the vacuum state) with finite particle number expectation. For such a normal state \( \omega \), there exists a density matrix \( \rho \), i.e., \( \rho \in \mathcal{L}^1(\mathcal{F}^\pm), \rho \geq 0, \operatorname{tr}_{\mathcal{F}^\pm}(\rho) = 1 \), such that
\[ \forall A \in \mathcal{A}^\pm, \quad \omega(A) = \operatorname{tr}_{\mathcal{F}^\pm}(\rho A) \quad \text{and} \quad \omega(\mathbb{1}) < \infty. \]

For bosons, we denote the set of these states by \( \mathcal{Z}^+ \). We restrict ourselves in the case of fermions to even states, i.e., for every odd \( n \in \mathbb{N} \) and any \( f_1, \ldots, f_n \in \mathfrak{h} \), we have \( \omega(a^*(f_1) \cdots a^*(f_n)) = 0 \), where \( a^*(f_j) \) denotes either a creation operator \( a^*(f_j) \) or an annihilation operator \( a(f_j) \). For fermions, the set of even, normal states with finite particle number expectation is denoted by \( \mathcal{Z}^- \). A state \( \omega \in \mathcal{Z}^\pm \) is called pure if there is a \( \Psi \in \mathcal{F}^\pm \), such that, for any \( A \in \mathcal{A}^\pm, \omega(A) = \langle \Psi, A\Psi \rangle_{\mathcal{F}^\pm} \).

We now define separately the notions of quasi-free states for bosons and fermions.

Quasi-free states for bosons

Definition 2.4. A state \( \omega \in \mathcal{Z}^+ \) is called quasi-free, shortly \( \omega \in \mathcal{Z}^+_q \), if there is a positive semi-definite operator \( h_\omega \) on \( \mathfrak{h} \), a \( \mathbb{R} \)-linear symplectomorphism \( T_\omega \) with respect to the symplectic form \( \operatorname{Im}(\cdot, \cdot)_\mathfrak{h} \), and \( f_\omega \in \mathfrak{h} \) such that, for every \( f \in \mathfrak{h} \),
\[ \omega(\mathbb{1} f) = \exp \left( 2i \operatorname{Im}(f_\omega, f)_\mathfrak{h} - \frac{1}{2} \langle T_\omega f, (1_\mathfrak{h} + h_\omega) T_\omega f \rangle_\mathfrak{h} \right). \]

The subset of pure quasi-free states is denoted by \( \mathcal{Z}^+_q \).

To link this notion of quasi-freeness to Wick’s theorem, we need the notion of centered states:

Definition 2.5. A centered state is a state \( \omega \in \mathcal{Z}^+ \) with
\[ \omega(a^*(f)) = 0 \]
for any \( f \in \mathfrak{h} \). We denote the set of all centered states by \( \mathcal{Z}^+_c \).
Note that the correlation functions $\omega(a^{\pi_1}(f_1) \ldots a^{\pi_N}(f_N))$ (where $a^{\pi_i}(f_i)$ is either a creation or annihilation operator) of a quasifree state may be non-vanishing even for odd values of $K$, unless $\omega$ is a centered quasifree state, i.e., $\omega \in Z^\mathrm{cfq}_+$. In this case, even correlation functions obey Wick’s theorem,

$$\omega(a^{\pi_1}(f_1) \ldots a^{\pi_{2N}}(f_{2N})) = \sum_{\pi \in \Pi_{2N}} \prod_{j=1}^{N} \omega(a^{\pi_{2j-1}}(f_{\pi(2j-1)})a^{\pi_{2j}}(f_{\pi(2j)})).$$

where $\Pi_{2N} \subseteq \Sigma_{2N}$ denotes the pairings of $2N$ objects. See below the definition of quasifree states for fermions for the definition of a pairing.

With this definition of quasifree ness, for bosons, only centered quasifree states fulfill Wick’s theorem.

**Definition 2.6.** A state $\omega \in Z^+$ is called coherent, $\omega \in Z^+_{\text{coh}}$, if there is a $f \in \mathfrak{h}$ such that

$$\forall A \in \mathfrak{A}^+, \omega(A) = [\Omega, \mathcal{W}^*_f A \mathcal{W}^*_f \Omega]_{\mathfrak{h}^+}.$$  

**Remark 2.7.** We have $Z^+_{\text{cfq}} \subseteq Z^+_{\text{coh}}$, $Z^+_{\text{coh}} \subseteq Z^+_{\text{pqf}} \subseteq Z^+_{\text{cfq}}$, and $Z^+_{\text{coh}} \cap Z^+_{\text{cen}} = \{ (\Omega, (\cdot) \Omega)_{\mathfrak{h}^+} \}$. 

**Quasifree states for fermions**

**Definition 2.8.** A state $\omega \in Z^-$ is called quasifree, shortly $\omega \in Z^-_{\text{qf}}$, if it fulfills Wick’s theorem, i.e., for every $N \in \mathbb{N}$ and any $f_1, \ldots, f_{2N} \in \mathfrak{h}$,

$$\omega(a^{\pi_1}(f_1) \ldots a^{\pi_{2N-1}}(f_{2N-1})) = 0 \quad \text{and} \quad \omega(a^{\pi_1}(f_1) \ldots a^{\pi_{2N}}(f_{2N})) = \sum_{\pi \in \Pi_{2N}} (-1)^{\pi} \prod_{j=1}^{N} \omega(a^{\pi_{2j-1}}(f_{\pi(2j-1)})a^{\pi_{2j}}(f_{\pi(2j)})).$$

where $a^{\pi_i}(f_i)$ denotes either a creation or an annihilation operator. The sum is taken over all pairings, that is, permutations $\pi \in \Sigma_{2N}$ satisfying

$$\pi(1) < \pi(3) < \ldots < \pi(2N-1) \quad \text{and, } \forall k \in \{1, 2, \ldots, N\}, \quad \pi(2k-1) < \pi(2k).$$

The subset of the pure quasifree states is denoted by $Z^\pm_{\text{pqf}}$. For any $N \in \mathbb{N}$ and any orthonormal vectors $\varphi_1, \ldots, \varphi_N \in \mathfrak{h}$, the vector $\varphi_1 \wedge \ldots \wedge \varphi_N := \sqrt{N!} S_N^- (\varphi_1 \otimes \ldots \otimes \varphi_N) \in \mathcal{F}^-$ is called Slater determinant and defines a pure quasifree state.

For both bosons and fermions

**Remark 2.9.** $Z^\pm_{\text{cfq}}$ and $Z^\pm_{\text{pqf}}$ are invariant under Bogoliubov and (in the case of bosons) Weyl transformations, i.e., the transform of a (pure) quasifree state is (pure) quasifree, as well.

### 3. One-particle and generalized one-particle density matrices

In Ref. 5, a generalized 1-pdm is defined for fermions on the space $\mathfrak{h} \oplus \mathfrak{h}$. We provide a definition of the generalized 1-pdm for both bosons and fermions. The definitions depend on the choice of the ONB of $\mathfrak{h}$, since we use complex conjugates of functions, as well as operators. We refer the reader to Ref. 18 for a basis independent formulation.

**Definition 2.10.** For any state $\omega \in Z^\pm$, we define the operators $\gamma_\omega$ and $\alpha_\omega$ on $\mathfrak{h}$, and $\tilde{\gamma}_\omega$ on $\mathfrak{h} \oplus \mathfrak{h}$ by their matrix elements, for $f, g, f_1, f_2, g_1, g_2 \in \mathfrak{h}$,

$$\langle f, \gamma_\omega g \rangle_\mathfrak{h} := \omega(a^*(g)a(f)), \quad \langle f, \alpha_\omega^* g \rangle_\mathfrak{h} := \omega(a^{\ast}(g)a^{\ast}(f)), \quad \text{and}$$

$$\langle (f_1 \oplus f_2), \tilde{\gamma}_\omega (g_1 \oplus g_2) \rangle_{\mathfrak{h} \oplus \mathfrak{h}} := \omega([a^*(g_1) + a(f_1)]\tilde{a}(f_2) + a^*(f_2)\tilde{a}(g_2))].$$

The operator $\gamma_\omega$ (resp. $\tilde{\gamma}_\omega$) is called the 1-pdm of $\omega$ (resp. the generalized 1-pdm of $\omega$).
Remark 2.11. The generalized 1-pdm $\tilde{\gamma}_\omega$ can be written in terms of $\gamma_\omega$ and $\alpha_\omega$ as

$$\tilde{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega \\ \alpha_\omega^* & \mathbb{1}_h \pm \overline{\gamma}_\omega \end{pmatrix}. $$

The 1-pdm $\gamma_\omega$ is self-adjoint and $\alpha_\omega^T = \pm \alpha_\omega$, i.e., $\alpha_\omega$ is symmetric for bosons and antisymmetric for fermions, where its transpose is $\alpha_\omega^T := \overline{\alpha_\omega}$.

The 1-pdm is a self-adjoint, positive semi-definite operator. It is trace class as

$$\text{tr}_h (\gamma_\omega) = \sum_{k=1}^\infty \langle \psi_k, \gamma_\omega \psi_k \rangle_h = \omega \left( \sum_{k=1}^\infty \alpha_k^* \alpha_k \right) = \omega \left( \mathbb{N} \right) < \infty. $$

Lemma 2.12. For any $\omega \in \mathit{Z}^+$, the generalized 1-pdm $\tilde{\gamma}_\omega$ as defined by (15) is a positive semi-definite operator on $h \oplus h$. In particular, it is self-adjoint.

In the case of fermions, it is bounded above by $\mathbb{1}_h \oplus \mathbb{1}_h$.

Proof. By setting $g_1 = f_1$ and $g_2 = f_2$, the first assertion is a consequence of (15) and the positivity of the corresponding state. We refer the reader to Ref. 5 for a proof of the bound by $\mathbb{1}_h \oplus \mathbb{1}_h$ in the case of fermions.

Therefore, the boson 1-pdm $\gamma$ is positive semi-definite, too. In the fermion case, $\gamma \leq \mathbb{1}_h$ also holds.

A consequence of Wick’s theorem is the following lemma.

Lemma 2.13. A centered quasifree state $\omega \in \mathit{Z}_\text{qf}^+$, or a quasifree state $\omega \in \mathit{Z}_\text{qf}^-$, is uniquely determined by its generalized 1-pdm $\tilde{\gamma}_\omega$.

Furthermore, the generalized 1-pdm transforms in a specific manner under Bogoliubov transformations:

Lemma 2.14. Let $\omega \in \mathit{Z}^\pm$ be a state with generalized 1-pdm $\tilde{\gamma} : h \oplus h \to h \oplus h$. For a Bogoliubov transformation $U : h \oplus h \to h \oplus h$ with unitary representation $\mathbb{U}_U : \mathcal{F}^\pm \to \mathcal{F}^\pm$, define $\omega_U$ by $\omega_U (A) := \omega (\mathbb{U}_U A \mathbb{U}_U^*)$ for any $A \in \mathcal{A}^\pm$. Then, the generalized 1-pdm $\tilde{\gamma}_U$ of the state $\omega_U$ is given by

$$\tilde{\gamma}_U = U^* \tilde{\gamma} U. $$

In the case of bosons, $\tilde{\gamma} S \tilde{\gamma} = -\tilde{\gamma}$ implies $\tilde{\gamma}_U S \tilde{\gamma}_U = -\tilde{\gamma}_U$. In the case of fermions, $\tilde{\gamma}_U^2 = \tilde{\gamma}$ implies $\tilde{\gamma}_U^2 = \tilde{\gamma}_U$.

Proof. We consider the matrix elements of $\tilde{\gamma}_U$. For the first assertion, we obtain

$$\langle (f_1 \oplus f_2), \tilde{\gamma}_U (g_1 \oplus g_2) \rangle_{h \oplus h} = \omega (\mathbb{U}_U [a^*(g_1) + a (\overline{g}_2)] \mathbb{U}_U^* \mathbb{U}_U [a(f_1) + a^*(\overline{f}_2)] \mathbb{U}_U^*)
= \omega (a^*[ug_1 + vg_2] + a(u\overline{g}_2 + v\overline{g}_1) \times [a(u f_1 + vf_2) + a^*(u \overline{f}_2 + v \overline{f}_1)])
= \langle U (f_1 \oplus f_2), \tilde{\gamma} U (g_1 \oplus g_2) \rangle_{h \oplus h}$$

for any $f_1, f_2, g_1, g_2 \in h$. Thus, (16) holds.

The assertion for bosons follows from (16) and $USU^* = S$:

$$\tilde{\gamma}_U S \tilde{\gamma}_U = U^* \tilde{\gamma} U SU^* \tilde{\gamma} U = U^* \tilde{\gamma} \tilde{\gamma} U = -U^* \tilde{\gamma} U = -\tilde{\gamma}_U. $$

The assertion for fermions follows from (16) and the unitarity of $U$: $\tilde{\gamma}_U^2 = U^* \tilde{\gamma} U U^* \tilde{\gamma} U = U^* \tilde{\gamma}^2 U$ and $\tilde{\gamma}^2 = \tilde{\gamma}$ yield $\tilde{\gamma}_U^2 = U^* \tilde{\gamma} U = \tilde{\gamma}_U$. □
4. Two-particle density matrix and representability

For systems with pair interactions, the formulation of the variational problem can be reduced by the notion of one- and two-particle density matrices.

**Definition 2.15.** The 2-pdm \( \Gamma_\omega : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h} \) of a state \( \omega \in \mathcal{Z}^\pm \) with \( \omega(\hat{N}^2) < \infty \) is defined by

\[
\forall f_j, g_j \in \mathfrak{h}, \quad \langle f_1 \otimes f_2, \Gamma_\omega (g_1 \otimes g_2) \rangle_{\mathfrak{h} \otimes \mathfrak{h}} := \omega(a^*(g_2)a^*(g_1) a(f_1)a(f_2)).
\]

The 2-pdm is a self-adjoint and positive semi-definite trace class operator, since

\[
\text{tr}_{\mathfrak{h} \otimes \mathfrak{h}} (\Gamma_\omega) = \omega(\hat{N}^2 - \hat{n}) < \infty
\]

and, for any \( \psi = \sum_{k,l=1}^\infty \mu_{kl} (\varphi_k \otimes \varphi_l) \in \mathfrak{h} \otimes \mathfrak{h} \) with \( (\mu_{kl})_{k,l=1}^\infty \in \ell^2(\mathbb{N}^2) \),

\[
\langle \psi, \Gamma_\omega \psi \rangle_{\mathfrak{h} \otimes \mathfrak{h}} = \sum_{i,j,k,l=1}^\infty \mu_{kl} \omega(a^*_k a^*_l a_j a_i) = \omega(PP^*) \geq 0,
\]

where \( P := \sum_{k,l=1}^\infty \mu_{kl} a^*_k a^*_l \). Furthermore, the 2-pdm is symmetric for bosons and antisymmetric for fermions, i.e., \( \Gamma_\omega \text{Ex} = \text{Ex} \Gamma_\omega = \pm \Gamma_\omega \). Here, the exchange operator \( \text{Ex} : \mathfrak{h} \otimes \mathfrak{h} \to \mathfrak{h} \otimes \mathfrak{h} \) is the linear map such that

\[
\text{Ex} (f \otimes g) := g \otimes f
\]

for any \( f, g \in \mathfrak{h} \). Summarizing the basic properties of the 1- and 2-pdm, we introduce the notions of admissibility and representability. (An outline of basic properties of the fermion 1- and 2-pdm can be found in Lemma 2.1 of Ref. 4.)

**Definition 2.16.** We call a pair \((\gamma, \Gamma)\) of operators on \( \mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h}) \) admissible if

(i) \( \Gamma \in L^1(\mathfrak{h} \otimes \mathfrak{h}) \) is symmetric for bosons resp. antisymmetric for fermions, i.e., \( \text{Ex} \Gamma = \Gamma \text{Ex} = \pm \Gamma \), and self-adjoint, and

(ii) \( \gamma \in L^1(\mathfrak{h}) \) is self-adjoint, positive semi-definite, and, in the case of fermions, \( \gamma \leq 1_\mathfrak{h} \).

Note that \( \text{tr}_\mathfrak{h}(\gamma) \) yields the particle number expectation value.

**Definition 2.17.** We say that the pair \((\gamma, \Gamma)\) of operators on \( \mathfrak{h} \times (\mathfrak{h} \otimes \mathfrak{h}) \), respectively, is representable if there is a state \( \omega \in \mathcal{Z}^\pm \) with \( \gamma_\omega = \gamma \) and \( \Gamma_\omega = \Gamma \). Necessary conditions on the pair \((\gamma, \Gamma)\) to be representable are called representability conditions.

In particular, every representable pair \((\gamma, \Gamma)\) is admissible.

So far, the definitions and statements are well established and can be found, for example, in Ref. 18, in Ref. 15 for bosons, and, in a version for fermions, in Ref. 5.

5. Further generalized one-particle density matrix and generalized two-particle density matrix for bosons

We further generalize the one- and the two-particle density matrices in the case of bosons. We begin with a further generalization of the 1-pdm on the space \( \mathfrak{h}_{\text{gen}} := \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C} \).
Definition 2.18. For any state $\omega \in \mathcal{Z}^+$, the further generalized 1-pdm $\hat{\gamma}_\omega : \mathcal{H}_\text{gen} \to \mathcal{H}_\text{gen}$ is defined by
\[
\langle G, \hat{\gamma}_\omega F \rangle_{\mathcal{H}_\text{gen}} := \omega \left( a^* (f_1) + a(\overline{f}_2) + \mu \right) \left[ a(g_1) + a^* (\overline{g}_2) + \overline{\mu} \right)
\]
for $F = f_1 \otimes f_2 \otimes \mu$ and $G = g_1 \otimes g_2 \otimes \nu \in \mathcal{H}_\text{gen}$.

Remark 2.19. We rewrite the further generalized 1-pdm $\hat{\gamma}_\omega$ as a $3 \times 3$-matrix
\[
\hat{\gamma}_\omega = \begin{pmatrix} \gamma_\omega & \alpha_\omega & b_\omega \\ \alpha^*_\omega & 1 + \overline{\gamma}_\omega & \overline{b}_\omega \\ b^*_\omega & \overline{b}^*_\omega & 1 \end{pmatrix}.
\]
Here, the first moment $b_\omega \in \mathfrak{h}$ and its dual element $b^*_\omega \in \mathfrak{h}^*$ are given by
\[
\langle g, b_\omega \rangle_{\mathfrak{h}} := \omega (a(g)) \quad \text{and} \quad b^*_\omega \cdot g \equiv (b_\omega, g)_{\mathfrak{h}} = \omega (a^*(g))
\]
for every $g \in \mathfrak{h}$. For the complex conjugate $\overline{b}_\omega$ of the wave function $b_\omega \in \mathfrak{h}$, we have \( \langle g, \overline{b}_\omega \rangle_{\mathfrak{h}} = \overline{\omega (a(g))} = \omega (a^*(g)) \).

Proposition 2.20. The further generalized 1-pdm is positive semi-definite and self-adjoint.

Proof. The self-adjointness is a direct consequence of (18). By setting $F = G$ in (17), $\hat{\gamma} \geq 0$ follows from the positivity of the state $\omega$. \qed

Lemma 2.21. Let $\hat{\gamma} = \left( \begin{array}{ccc} \gamma & \alpha & b \\ a^* & 1 \pm b & \overline{\gamma} \\ b^* & \overline{\alpha} & 1 \end{array} \right) : \mathcal{H}_\text{gen} \to \mathcal{H}_\text{gen}$ be a positive semi-definite trace class operator with $b \in \mathfrak{h}$, $\gamma \in \mathcal{L}^1(\mathfrak{h})$, and $\alpha \in \mathcal{L}^2(\mathfrak{h})$. Then, there is a unique quasifree state $\omega$ that has $\hat{\gamma}$ as its further generalized 1-pdm.

In particular, for any positive semi-definite trace class operator $\hat{\gamma} = \left( \begin{array}{ccc} \gamma & \alpha & b \\ a^* & 1 \pm b & \overline{\gamma} \\ b^* & \overline{\alpha} & 1 \end{array} \right) : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ with $\gamma \in \mathcal{L}^1(\mathfrak{h})$ and $\alpha \in \mathcal{L}^2(\mathfrak{h})$, there is an $\omega \in \mathcal{Z}^+$ with $\hat{\gamma}_\omega = \hat{\gamma}$. \qed

Proof. The second part is a consequence of Theorem 11.4 in Ref. 18 or Theorem 1.6 (i) in Ref. 15. The first part follows from the second part due to the fact that a non-centered state with first moment $b \in \mathfrak{h}$ is completely characterized by a Weyl operator $\mathcal{W}_b$ and the centered state $\omega_0$ defined by $\omega_0 (A) := \omega (\mathcal{W}^*_b A \mathcal{W}_b)$ for any $A \in \mathcal{A}^+$. \qed

Analogously, assuming $\omega (\mathcal{N}^2) < \infty$, we define a generalized two-particle density matrix $\hat{\Gamma}$ on
\[
\mathcal{H}_\text{sim} := \left( \bigoplus_{n=1}^4 \mathfrak{h} \otimes \mathfrak{h} \right) \oplus \left( \bigoplus_{n=1}^2 \mathfrak{h} \right) \oplus \mathbb{C}.
\]
Technically, the generalized 2-pdm should be defined on
\[
\mathcal{H}_\text{gen} \otimes \mathcal{H}_\text{gen} \cong \left( \bigoplus_{n=1}^4 \mathfrak{h} \otimes \mathfrak{h} \right) \oplus \left( \bigoplus_{n=1}^4 \mathfrak{h} \right) \oplus \mathbb{C}.
\]
It suffices, however, to consider $\mathcal{H}_\text{sim}$, since for any polynomial of degree 1 in annihilation and creation operators there are an ONB $\{\varphi_k\}_{k=1}^N$ of $\mathfrak{h}$, a $N \in \mathbb{N}$, and coefficients $\mu_k, v_k, \sigma_k, \tau_k, \tilde{\mu}_k, \tilde{v}_k \in \mathbb{C}, k = 1, \ldots, N$, such that
\[
\sum_{k=1}^N (\mu_k a_k^* + v_k a_k + \sigma_k a_k + \tau_k a_k^*) = \sum_{k=1}^N (\tilde{\mu}_k a_k^* + \tilde{v}_k a_k).
\]
For any $M \in \mathbb{N}$ and a given ONB $\{\varphi_k\}_{k=1}^N$ of $\mathfrak{h}$, we set $F := (F_1, F_2, F_3, F_4)^T, G := (G_1, G_2, G_3, G_4)^T, f := (f_1, f_2)^T$, and $g := (g_1, g_2)^T$ with $F_i := \sum_{k=1}^M \mu_k^{(i)} (\varphi_k \otimes \varphi_k), G_i := \sum_{k=1}^M \nu_k^{(i)} (\varphi_k \otimes \varphi_k)$ and $\varphi_k \in \mathcal{H}_\text{sim}$.
\[ \mathfrak{h} \otimes \mathfrak{h}, \text{ and } f_j := \sum_{k=1}^{M} \mu_k^{(j)} \psi_k, \quad g_j := \sum_{k=1}^{M} \nu_k^{(j)} \psi_k \in \mathfrak{h}, \text{ where the coefficients } \mu_k^{(j)}, \nu_k^{(j)} \in \mathbb{C}, \quad k, j \in \{1, \ldots, M\}. \]

Then, we define the polynomials \( P_1 \) and \( P_2 \) by

\[
P_1(f) := \sum_{k=1}^{M} \left( \mu_k^{(1)} a_k^* + P_k^{(2)} a_k \right),
\]

\[
P_2(F) := \sum_{k,j=1}^{M} \left( \mu_k^{(1)} a_k^* a_j^* + \mu_k^{(2)} a_k^* a_j + \mu_k^{(3)} a_k a_j^* + \mu_k^{(4)} a_k a_j \right).
\]

**Definition 2.22.** The generalized 2-pdm \( \tilde{\Gamma}_\omega \) is defined by

\[
\left( \begin{array}{c} G \\ \mu \\ f \end{array} \right), \tilde{\Gamma}_\omega \left( \begin{array}{c} F \\ g \\ v \end{array} \right) := \omega \left( (P_2(F) + P_1(f) + v) (P_1^*(g) + P_2^*(F) + \mu) \right)
\]

for any \( F, G \in \bigoplus_{\mu, \nu} (\mathfrak{h} \otimes \mathfrak{h}) \) with \( \sum_{k=1}^{\infty} \mu_k^{(3)} \), \( \sum_{k=1}^{\infty} \nu_k^{(3)} < \infty \), \( f, g \in \mathfrak{h} \otimes \mathfrak{h} \), and \( \mu, v \in \mathbb{C} \) as an operator on \( \mathfrak{h}_\text{adm} \). The polynomials \( P_1 \) and \( P_2 \) are of the form specified above.

As for the generalized 1-pdm, an easy consequence of the definition are the following properties.

**Proposition 2.23.** The generalized 2-pdm is self-adjoint and positive semi-definite.

In the Appendix, we establish a relation between the generalized 2-pdm and bosonic representability conditions for systems, in which the particle number is not conserved.

### B. Bogoliubov–Hartree–Fock theory

#### 1. Boson Bogoliubov–Hartree–Fock theory

For bosons, the number of particles in most physically relevant models is not fixed. As, for instance, in a system of photons interacting with an electron, photons can appear or disappear, depending on what is energetically favorable. Thus, the particle number should not be fixed in the variational process yielding the ground state energy \( E_{\text{gs}} := \inf \{ \sigma(\mathbb{H}) \} \). This approach is called grand canonical formalism. By the Rayleigh–Ritz principle, the ground state energy (as well as the ground state) is determined by

\[
E_{\text{gs}} = \inf \left\{ \omega(\mathbb{H}) \mid \omega \in \mathcal{Z}^+ \right\}.
\]

In the BHF theory, the variation is restricted to quasifree states

\[
E_{\text{BHF}} := \inf \left\{ \omega(\mathbb{H}) \mid \omega \in \mathcal{Z}^+_\text{qf} \right\}.
\]

The BHF energy \( E_{\text{BHF}} \) is an upper bound to the ground state energy \( E_{\text{gs}} \). Note that, unlike the common definitions of quasifreeness, our quasifree states are not necessarily centered. Since a quasifree state is uniquely determined by its further generalized 1-pdm \( \tilde{\gamma}_\omega \), there is an energy functional \( \mathcal{E}_{\text{BHF}} : \mathcal{D}(\mathcal{E}_{\text{BHF}}) \rightarrow \mathbb{C} \), \( \mathcal{D}(\mathcal{E}_{\text{BHF}}) \subseteq \mathcal{B}(\mathfrak{h} \otimes \mathfrak{h} \otimes \mathbb{C}) \), such that \( \omega(\mathbb{H}) = \mathcal{E}_{\text{BHF}}(\tilde{\gamma}_\omega) \). Thus, the BHF energy is rewritten as

\[
E_{\text{BHF}} = \inf \left\{ \mathcal{E}_{\text{BHF}}(\tilde{\gamma}_\omega) \mid \omega \in \mathcal{Z}^+_\text{qf} \right\} = \inf \left\{ \mathcal{E}_{\text{BHF}}(\tilde{\gamma}) \mid \tilde{\gamma} \geq 0, \, \text{tr}_{\mathfrak{h}}(\gamma) < \infty \right\}.
\]

The second equality is a consequence of Lemma 2.21: On the one hand, any quasifree state \( \omega \) with first moment \( b \) is linked to a unique centered quasifree state via the Weyl transformation \( W_b \). On the other hand, any positive semi-definite operator \( \tilde{\gamma} \) fulfilling \( \text{tr}(\gamma) < \infty \) is the generalized 1-pdm of a centered quasifree state, cf. Ref. 15.
2. Fermion Bogoliubov–Hartree–Fock theory

For a typical fermion system, assume $U : \mathbb{R}^3 \to \mathbb{R}$ to be an external potential and $V : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ a pair interaction. There are multiplication operators associated to these potentials which we also denote by $U$ and $V$, respectively. With the Laplace operator $\Delta$, the Hamiltonian of the system is given by

$$H_N := \sum_{i=1}^{N} [-\Delta_i - U(x_i)] + \sum_{1 \leq i < j \leq N} V(x_i, x_j),$$

where $x_i \in \mathbb{R}^3$, $1 \leq i \leq N$. We only allow potentials for which $H_N$ is defined as a self-adjoint operator on a dense domain $\mathcal{D}_N$ and is bounded below. The second quantization of this Hamiltonian is

$$\mathbb{H} = \sum_{i,j=1}^{\infty} h_{ij} a_i^* a_j + \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} V_{ij,kl} a_i^* a_j^* a_k a_l,$$

where the one-particle operator $h$ and the interaction operator are given by

$$h_{ij} := \langle \psi_i, (-\Delta - U) \psi_j \rangle_h \quad \text{and} \quad V_{ij,kl} := \langle \psi_i \otimes \psi_j, V(\psi_k \otimes \psi_l) \rangle_{h \otimes h}$$

for any elements of a given ONB $\{\psi_i\}_{i=1}^{\infty}$ of $h$ with $\|\nabla \psi_i\|_h < \infty$. The Hamiltonian $H_N$ is the restriction of $\mathbb{H}$ to the $N$-particle Fock space $S_N^N h^{\otimes N}$. Note that the Hamiltonians considered below are not necessarily of the form (20): The Hamiltonian $\mathbb{H}$ has to be simply self-adjoint and bounded below.

If we do not assume the dynamics to conserve the particle number (i.e., in the grand canonical picture), the ground state energy of the $N$-particle system is determined by the Rayleigh–Ritz principle: $E_{gs} = \inf \{ \langle \omega(\mathbb{H}) \rangle \omega \in \mathcal{Z}^{-} \}$. Using the energy functional $E(\gamma, \Gamma) := \operatorname{tr}_h(h \gamma) + \frac{1}{2} \operatorname{tr}_{h \otimes h}(V \Gamma)$, this can be re-expressed as

$$E_{gs} = \inf \{ E(\gamma, \Gamma) \ | \ (\gamma, \Gamma) \text{ is representable} \}.$$

Here, the problem of representability arises, i.e., a classification of all representable operator pairs on $h \times (h \otimes h)$. In order to obtain an upper bound to $E_{gs}$, the variation is restricted to quasifree states which yields the Bogoliubov–Hartree–Fock energy

$$E_{BHF} := \inf \{ \omega(\mathbb{H}) \ | \ \omega \in \mathcal{Z}_{qf} \} = \inf \{ E_{BHF}(\mathcal{F}) \ | \ \mathcal{F} \geq 0, \ \operatorname{tr}_h(\mathcal{F}) < \infty \}.$$

For any quasifree state $\omega$, the Bogoliubov–Hartree–Fock functional $E_{BHF}$ is given by $E_{BHF}(\mathcal{F}) := \omega(\mathbb{H})$, where $\mathcal{F}$ is the generalized 1-pdm of $\omega$.

III. VARIATION OVER PURE QUASIFREE STATES AND BOGOLIUOV–HARTREE–FOCK ENERGY

For bosons, Theorem 1.2 in Ref. 3 states for the Pauli–Fierz model that the Bogoliubov–Hartree–Fock energy coincides with the infimum of the energy functional for a variation over pure quasifree states. We prove a more general statement, which holds for bosons, as well as for fermions, and generalizes Lieb’s variational principle. Our main result is

**Theorem 3.1.** Assume the Hamiltonian $\mathbb{H}$ on $\mathcal{F}^\pm$ to be bounded below. Then,

$$E_{BHF} = \inf \{ \omega(\mathbb{H}) \ | \ \omega \in \mathcal{Z}_{pqf}^\pm \} := E_{BHF}^{\text{pure}}.$$  

We recall that $\mathcal{Z}_{pqf}^\pm$ denotes the set of pure quasifree states and that, for bosons, quasifree states are in general non-centered. We show the statement for bosons and fermions separately.

**Remark 3.2.** Although we do not prove it here, we believe that, at least for a smaller class of Hamiltonians, the existence of a quasifree minimizer implies the existence of a pure quasifree
minimizer. Additional assumptions on the Hamiltonian, like a coercivity property and the existence of a gap above the ground state energy, seem sufficient to ensure this.

A. Bosons

In order to prove the theorem, we need some properties of quasifree and pure quasifree states. To this end, we give a characterization of quasifree and pure quasifree states using the Bogoliubov and the Weyl transformation.

**Lemma 3.3.** For any quasifree density matrix \( \rho \), there are a positive semi-definite operator \( C \in \mathcal{L}^1(\mathfrak{h}) \) with \( \|C\|_{\mathfrak{h}(\mathfrak{h})} < 1 \) and second quantization \( \Gamma(C) := \bigoplus_{n=0}^{\infty} C^\otimes_n \), a boson Bogoliubov transformation with unitary implementation \( U \), and \( f \in \mathfrak{h} \) such that

\[
\rho = \mathbb{W}_f U \frac{\Gamma(C)}{\text{tr}_{f^-}(\Gamma(C))} U^* \mathbb{W}_f^*.
\]

If, in addition, the density matrix is pure, it is of the form \( \mathbb{W}_f U |\Omega\rangle \langle \Omega| U^* \mathbb{W}_f^* \), where we used the Dirac bra-ket notation.

This lemma is a consequence of Lemma 3.1 in Ref. 3. Note that, for a centered quasifree density matrix, \( f = 0 \) and, hence, \( \mathbb{W}_f = 1_{f^-} \) in Lemma 3.3.

**Proof of Theorem 3.1 for bosons.** Without loss of generality, we assume the Hamiltonian to be positive semi-definite. If \( \mathbb{H} \) is bounded below, there is a constant \( \mu \geq 0 \) such that \( \mathbb{H}_0 := \mathbb{H} + \mu 1_{f^-} \geq 0 \). Considering \( \mathbb{H}_0 \) instead of \( \mathbb{H} \) just adds the constant \( \mu \) to both \( E_{\text{BHF}} \) and \( E_{\text{BHF}}^\text{pure} \).

The inequality

\[
E_{\text{BHF}} = \inf \left\{ \omega(\mathbb{H}) \middle| \omega \in \mathbb{Z}_{\text{qf}}^+ \right\} \leq \inf \left\{ \omega(\mathbb{H}) \middle| \omega \in \mathbb{Z}_{\text{qf}}^+ \right\} = E_{\text{BHF}}^\text{pure}
\]

follows from the definition of the BHF energy, since the variation is restricted to the proper subset \( \mathbb{Z}_{\text{qf}}^+ \subseteq \mathbb{Z}_{\text{qf}}^+ \). The proof is complete if we show that \( \omega(\mathbb{H}) \geq E_{\text{BHF}}^\text{pure} \) for any quasifree state \( \omega \in \mathbb{Z}_{\text{qf}}^+ \).

Let \( \omega \in \mathbb{Z}_{\text{qf}}^+ \) with \( \omega(\mathbb{H}) < \infty \) and denote the corresponding density matrix by \( \rho \). Then,

\[
\omega(\mathbb{H}) = \text{tr}_{f^-}(\rho^\frac{1}{2} \mathbb{H} \rho^\frac{1}{2}) = \text{tr}_{f^-}(\rho^\frac{1}{2} \mathbb{H} \rho^\frac{1}{2})(\mathbb{H}^\frac{1}{2} \rho^\frac{1}{2}),
\]

since \( \mathbb{H} \geq 0 \). Therefore, \( \rho^\frac{1}{2} \mathbb{H} \rho^\frac{1}{2} \) is Hilbert–Schmidt and we obtain by the cyclicity of the trace

\[
\text{tr}_{f^-}(\rho^\frac{1}{2} \mathbb{H} \rho^\frac{1}{2})(\mathbb{H}^\frac{1}{2} \rho^\frac{1}{2}) = \text{tr}_{f^-}(\mathbb{H}^\frac{1}{2} \rho \mathbb{H}^\frac{1}{2}).
\]

Since \( \mathbb{H} \) is self-adjoint, there is an ONB \( (\Psi_k)_{k=1}^\infty \) of \( \mathcal{F}^+ \), such that \( \Psi_k \in \mathcal{D}(\mathbb{H}) \) for any \( k \in \mathbb{N} \). Then,

\[
\text{tr}_{f^-}(\mathbb{H}^\frac{1}{2} \rho \mathbb{H}^\frac{1}{2}) = \sum_{k=1}^{\infty} \langle \mathbb{H}^\frac{1}{2} \Psi_k, \rho \mathbb{H}^\frac{1}{2} \Psi_k \rangle_{f^-}.
\]

By Lemma 3.3, the positive semi-definite operator \( \rho \) can be written as \( \rho = \kappa \kappa^* \), where

\[
\kappa := \mathbb{W}_f U [\text{tr}_{f^-}(\Gamma(C))]^{-\frac{1}{2}} \Gamma(C)^{\frac{1}{2}}
\]

with some \( f \in \mathfrak{h} \), a Bogoliubov transformation with unitary implementation \( U \), and some \( C \in \mathcal{L}^1(\mathfrak{h}) \), \( C \geq 0 \), \( \|C\|_{\mathfrak{h}(\mathfrak{h})} < 1 \). Hence,

\[
\omega(\mathbb{H}) = \sum_{k=1}^{\infty} \left\| \kappa^* \mathbb{H}^\frac{1}{2} \Psi_k \right\|_{f^+}^2.
\]  

We continue by introducing a resolution of the identity with coherent states. To this end, we consider an increasing sequence of \( n \)-dimensional Hilbert spaces \( \mathfrak{h}_n \subseteq \mathfrak{h}_{n+1} \subseteq \mathfrak{h} \), \( n \in \mathbb{N} \), with \( \bigcup_{n \in \mathbb{N}} \mathfrak{h}_n = \mathfrak{h} \) and \( C \mathfrak{h}_n \subseteq \mathfrak{h}_n \). For any \( n \)-dimensional Hilbert space \( \mathfrak{h}_n \), there is an isometric isomorphism \( I : \mathfrak{h}_n \to \mathbb{C}^n \). We define the measure \( d\mu_n(z^{(n)}) \) on \( \mathfrak{h}_n \) by \( \int_{\mathfrak{h}_n} d\mu_n(z^{(n)}) f(z^{(n)}) := \int_{\mathbb{C}^n} \frac{d^nd\omega}{\pi} f(Iz^{(n)}) \), where \( x := \text{Re}(Iz^{(n)}) \), \( y := \text{Im}(Iz^{(n)}) \). For any \( n \in \mathbb{N} \), we have \( \mathfrak{h} = \mathfrak{h}_n \oplus \mathfrak{h}_n^\perp \), where \( \mathfrak{h}_n^\perp \) denotes the
orthogonal complement of $h_n$ in $h$. Moreover, $\mathcal{F}^+ \cong \mathcal{F}^+[h_n] \otimes \mathcal{F}^+[h_n^\perp]$ and $\Omega = \Omega_n \otimes \Omega_n^\perp$ with $\Omega_n \in \mathcal{F}^+[h_n]$ and $\Omega_n^\perp \in \mathcal{F}^+[h_n^\perp]$. For every $n \in \mathbb{N}$, the projections $|\mathbb{W}_{\mathcal{C}^n_n} \Omega \rangle \langle \mathbb{W}_{\mathcal{C}^n_n} \Omega |$, $z^{(n)} \in h_n$, satisfy

$$1_{\mathcal{F}^+[h_n]} \otimes \Omega^+_n |\mathbb{W}_{\mathcal{C}^n_n} \Omega \rangle = \int_{h_n} d\mu_n(z^{(n)}) |\mathbb{W}_{\mathcal{C}^n_n} \Omega \rangle \langle \mathbb{W}_{\mathcal{C}^n_n} \Omega |$$

see, e.g., Refs. 6 and 10. Consequently,

$$\| \Psi \|^2 = \lim_{n \to \infty} \int_{h_n} d\mu_n(z^{(n)}) |\langle \Psi, \mathbb{W}_{\mathcal{C}^n_n} \Omega \rangle|^2$$

for any $\Psi \in \mathcal{F}^+$. Thus, the right hand side of (21) is rewritten as

$$\sum_{k=1}^\infty \left\| \kappa \frac{H}{\Omega_i} \psi^k \right\|^2 = \sum_{k=1}^\infty \lim_{n \to \infty} \int_{h_n} d\mu_n(z^{(n)}) \left| \left\langle \kappa \frac{H}{\Omega_i} \psi^k, \kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega \right\rangle \right|^2.$$

The sequence $k \mapsto \int_{h_n} d\mu_n(z^{(n)}) \left| \left\langle \frac{H}{\Omega_i} \psi^k, \kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega \right\rangle \right|^2$ is monotonously increasing. Therefore, the summation over $k$ and the limit $n \to \infty$ can be exchanged by the monotone convergence theorem, where the summation is considered as an integral with the counting measure. Thus, we obtain

$$\omega(\mathbb{H}) = \lim_{n \to \infty} \sum_{k=1}^\infty \int_{h_n} d\mu_n(z^{(n)}) \left| \left\langle \kappa \frac{H}{\Omega_i} \psi^k, \kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega \right\rangle \right|^2.$$

Afterwards, Fubini’s theorem yields

$$\omega(\mathbb{H}) = \lim_{n \to \infty} \int_{h_n} d\mu_n(z^{(n)}) \sum_{k=1}^\infty \left| \left\langle \kappa \frac{H}{\Omega_i} \psi^k, \kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega \right\rangle \right|^2 = \lim_{n \to \infty} \int_{h_n} d\mu_n(z^{(n)}) \left( \kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega, \mathbb{W}_{\mathcal{C}^n_n} \Omega \right)_{\mathcal{F}^+}.$$

Now, we observe that, due to $\mathbb{W}_{\mathcal{C}^n_n} \Omega = \exp \left( -\frac{\|z^{(n)}\|^2}{2} \sum_{m=0}^\infty (z^{(n)}) \otimes m / \sqrt{m!} \right)$,

$$\kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega = \mathbb{W}_f \cup \left( \text{tr}_{\mathcal{F}^+}(\Gamma(C)) \right)^{-1/2} \Gamma(C^{1/2}) \mathbb{W}\mathcal{C}^n_n \Omega \subset \mathbb{W}_f \cup \mathbb{W}\mathcal{C}^n_n \Omega.$$

The Bogoliubov transformation $U$ and the Weyl transformation $\mathbb{W}_{\mathcal{C}^n_n}$ can be commuted (up to a transformation of the argument of the Weyl transformation) and we obtain

$$\kappa \mathbb{W}_{\mathcal{C}^n_n} \Omega = \nu_{\mathcal{C}^n, g}(z^{(n)}) \mathbb{W}_g \cup \mathbb{W}\mathcal{C}^n_n \Omega$$

for some $g \in h$ and $\nu_{\mathcal{C}^n, g}(z^{(n)}) \in \mathbb{C}$ with $|\nu_{\mathcal{C}^n, g}(z^{(n)})|^2 = \left( \text{tr}_{\mathcal{F}^+}(\Gamma(C)) \right)^{-1} \exp \left( -\frac{\|C^{1/2}z^{(n)}\|^2 - \|z^{(n)}\|^2}{2} \right)$. From the proof of Lemma 3.7 in Ref. 3, we conclude

$$\int_{h_n} d\mu_n(z^{(n)}) \left| \nu_{\mathcal{C}^n, g}(z^{(n)}) \right|^2 = \left( \text{tr}_{\mathcal{F}^+}(\Gamma(C)) \right)^{-1} \text{tr}_{\mathcal{F}^+}(\Gamma(C \mid_{h_n})), $$

which converges to 1 as $n \to \infty$ (see proof of Theorem 3.5 in Ref. 3). By Lemma 3.3, $\mathbb{W}_g \cup \mathbb{W}\mathcal{C}^n_n \Omega$ defines a pure quasifree state and, consequently,

$$\omega(\mathbb{H}) \geq E_{\text{BHFF}} \lim_{n \to \infty} \int_{h_n} d\mu_n(z^{(n)}) \left| \nu_{\mathcal{C}^n, g}(z^{(n)}) \right|^2 = E_{\text{BHFF}}^\text{pure},$$

which completes the proof.
B. Fermions

Before we prove Theorem 3.1 for fermions, we need two preparatory lemmas.

**Lemma 3.4.** Let \( \omega \in Z_q \) with density matrix \( \rho \). Then, there is a decomposition \( \mathfrak{h} = \mathfrak{h}_S \oplus 1 \mathfrak{h}_T \) with \( n := \dim(\mathfrak{h}_S) < \infty \), a positive semi-definite trace class operator \( B \in \mathcal{B}(\mathfrak{h}_T) \), and a fermion Bogoliubov transformation \( U \) with unitary implementation \( U_B \) such that

\[
\rho = U_B \left( (\langle \psi_1 \ldots \psi_n \rangle \langle \psi_1 \ldots \psi_n \rangle) \otimes (\text{tr}_{-} (\Gamma(B)))^{-1} \Gamma(B) \right) U_B^*,
\]

for any ONB \( \{ \psi_k \}_{k=1}^{n} \) of \( \mathfrak{h}_S \).

**Proof.** It is known that there are fermion Bogoliubov transformations \( U \) such that the generalized 1-pdm of \( \rho_U := \mathcal{U}_B^* \rho \mathcal{U}_B \) is of the form

\[
\gamma_U = \begin{pmatrix} \gamma_U & 0 \\ 0 & \mathbb{I}_n - \gamma_U \end{pmatrix}
\]

for some \( 0 \leq \gamma_U \leq \mathbb{I}_n \) with \( \text{tr}_S (\gamma_U) < \infty \), see, e.g., Theorem 2.3 in Ref. 5. Let \( \mathfrak{h}_S \) be the eigenspace of \( \gamma_U \) associated to the eigenvalue \( 1 \) with dimension \( n < \infty \) and \( \mathfrak{h}_T \) its orthogonal complement. Then, \( \gamma_U = P_S + \gamma_T \), where \( P_S \) is the orthogonal projection on \( \mathfrak{h}_S \) and \( \gamma_T \) the restriction of \( \gamma_U \) to \( \mathfrak{h}_T \). Note that \( \gamma_T \) satisfies \( \gamma_T \subseteq \ker(\gamma_T) \), \( \gamma_T \mathfrak{h}_T \subseteq \mathfrak{h}_T \), and \( 0 \leq \gamma_T \leq \mu \Gamma_0 \) for some \( 0 < \mu < 1 \). Let \( \varphi_1, \ldots, \varphi_n \) be an ONB of \( \mathfrak{h}_S \). Moreover, let

\[
\gamma := \rho_U := \mathcal{U}_B^* \rho \mathcal{U}_B \text{ is of the form (22)}
\]

with \( B := (\gamma_T)^{-1} (\mathbb{I}_{\mathfrak{h}_T} - \gamma_T)^{-1} \). In order to show that \( \rho' = \rho_U \), it is sufficient to observe that \( \rho' \) defines a quasifree state \( \omega' \) and \( \gamma_U' = \gamma_U \) from (23), since quasifree states are characterized by their general 1-pdm, see Ref. 5. Note that we implicitly used the decomposition \( \mathcal{F}^- \cong \mathcal{F}^- [\mathfrak{h}_S] \otimes \mathcal{F}^- [\mathfrak{h}_T] \).

**Remark 3.5.** For any positive semi-definite trace class operator \( B \in \mathcal{B}(\mathfrak{h}_T) \), there are an ONB \( \{ \phi_k \}_{k=1}^{n} \) of \( \mathfrak{h}_T \) and coefficients \( (b_k)_{k=1}^{n} \) such that \( B = \sum_{k=1}^{n} b_k \langle \phi_k | \phi_k \rangle \). Thus,

\[
\text{tr}_{-} (\Gamma(B)) = \text{tr}_{-} \left( \bigotimes_{k=1}^{n} \Gamma(b_k) \right) = \prod_{k=1}^{n} \text{tr}_{-} (\Gamma(b_k)) = \prod_{k=1}^{n} (1 + b_k)
\]

which converges due to \( \sum_{k=1}^{n} b_k < \infty \). Here, \( \Gamma(b_k) \) should be understood as the second quantized operator \( \Gamma(b_k) \langle \phi_k | \phi_k \rangle \) on \( \mathcal{F}^- [\mathbb{C} \phi_k] \).

**Lemma 3.6.** Let \( \omega \in Z_q \) with density matrix \( \rho \). Then, there is a sequence \( (\rho_k)_{k=1}^{\infty} \) of pure quasifree density matrices and \( (\lambda_k)_{k=1}^{\infty} \in [0, \infty) \) with \( \sum_{k=1}^{\infty} \lambda_k < \infty \) such that

\[
\langle \Psi_1, \rho \Psi_2 \rangle_{\mathcal{F}^-} = \lim_{n \to \infty} \langle \Psi_1, \sum_{k=1}^{n} \lambda_k \rho_k \Psi_2 \rangle_{\mathcal{F}^-}
\]

for any \( \Psi_1, \Psi_2 \in \mathcal{F}^- \). That is, every quasifree state is a convex combination of pure quasifree states.

**Proof.** From Lemma 3.4, we know that every quasifree density matrix is of the form (22) and we use the notation specified there in the following. We complete \( \{ \psi_k \}_{k=1}^{\infty} \) to an ONB \( \{ \phi_k \}_{k=1}^{\infty} \) of \( \mathfrak{h} \), where \( \{ \psi_k \}_{k=0}^{\infty} \) is an ONB of \( \mathfrak{h}_T \). Then,

\[
\langle \Psi, \Phi \rangle_{\mathcal{F}^-} = \lim_{N \to \infty} \lim_{M \to \infty} \sum_{k=0}^{N} \sum_{1 \leq i_1 < \ldots < i_k \leq M} \langle \Psi, \psi_{i_1} \ldots \psi_{i_k} \rangle_{\mathcal{F}^-} \langle \phi_{i_1} \ldots \phi_{i_k}, \Phi \rangle_{\mathcal{F}^-}
\]

for any \( \Phi, \Phi \in \mathcal{F}^- \).
for any $\Psi, \Phi \in \mathcal{F}^-$. Choosing the ONB $\{\psi_k\}_{k=m+1}^{\infty}$ of $\mathfrak{h}_{\Psi}$ such that $B$ is diagonalized and using (24), we obtain in the weak sense

\[
\kappa^2 := \left( |\varphi_1 \wedge \ldots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \ldots \wedge \varphi_n| \otimes [\text{tr}_{\mathcal{F}^-}(\Gamma(B))]^{-\frac{1}{2}} \Gamma(B^{\frac{1}{2}}) \right)^2
\]

\[
= \lim_{M,N \to \infty} \sum_{k=n}^{N} \sum_{n+1\leq i_1 < \ldots < i_k \leq M} (|\varphi_1 \wedge \ldots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \ldots \wedge \varphi_n|) \\
\otimes \left( \frac{\Gamma(B^{\frac{1}{2}})}{[\text{tr}_{\mathcal{F}^-}(\Gamma(B))]^{\frac{1}{2}}} |\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}\rangle \langle \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}| \frac{\Gamma(B^{\frac{1}{2}})}{[\text{tr}_{\mathcal{F}^-}(\Gamma(B))]^{\frac{1}{2}}} \right).
\]

(We interpret the case $k = n$ in the sum as giving $|\varphi_1 \wedge \ldots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \ldots \wedge \varphi_n|$.) This can be written as

\[
\kappa^2 = (\text{tr}_{\mathcal{F}^-}(\Gamma(B)))^{-1} \lim_{M,N \to \infty} \sum_{k=n}^{N} \sum_{n+1\leq i_1 < \ldots < i_k \leq M} (|\varphi_1 \wedge \ldots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \ldots \wedge \varphi_n|) \\
\otimes |B^{1/2}_{\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}} \varphi_{i_1} \wedge \ldots \wedge B^{1/2}_{\varphi_{i_k}}\varphi_{i_k}\rangle \langle B^{1/2}_{\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}} \varphi_{i_1} \wedge \ldots \wedge B^{1/2}_{\varphi_{i_k}}\varphi_{i_k}| \\
= (\text{tr}_{\mathcal{F}^-}(\Gamma(B)))^{-1} \lim_{M,N \to \infty} \sum_{k=n}^{N} \sum_{n+1\leq i_1 < \ldots < i_k \leq M} \langle \varphi_1 \wedge \ldots \wedge \varphi_n | B^{1/2}_{\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}} \varphi_{i_1} \wedge \ldots \wedge B^{1/2}_{\varphi_{i_k}}\varphi_{i_k} \rangle \\

\langle \varphi_1 \wedge \ldots \wedge \varphi_n | B^{1/2}_{\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}} \varphi_{i_1} \wedge \ldots \wedge B^{1/2}_{\varphi_{i_k}}\varphi_{i_k} \rangle.
\]

Each operator $|\varphi_1 \wedge \ldots \wedge \varphi_n | B^{1/2}_{\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_k}} \varphi_{i_1} \wedge \ldots \wedge B^{1/2}_{\varphi_{i_k}}\varphi_{i_k}$ is either equal to zero or a pure quasifree density matrix (up to a normalization constant). Finally, a pure quasifree density matrix conjugated by a Bogoliubov transformation is a pure quasifree state, too, which completes the proof. \hfill \Box

Now, we are prepared to prove Theorem 3.1 for fermions. Since the proof is, to a large extent, similar to the proof of Theorem 3.1 for bosons, we only give details where there are differences.

**Proof of Theorem 3.1 for fermions.** Again, without loss of generality, we assume that the Hamiltonian is positive semi-definite. As for bosons, the inequality

\[
E_{\text{BHF}} = \inf \left\{ \omega(\mathbb{H}) \mid \omega \in Z_{\Psi}^- \right\} \leq \inf \left\{ \omega(\mathbb{H}) \mid \omega \in Z_{\Psi}^{\text{pure}} \right\} = E_{\text{BHF}}^{\text{pure}}
\]

is immediate. Thus, we show $\omega(\mathbb{H}) \geq E_{\text{BHF}}^{\text{pure}}$ for any $\omega \in Z_{\Psi}^-$. Let $\omega \in Z_{\Psi}^-$ with $\omega(\mathbb{H}) < \infty$ and denote the corresponding density matrix by $\rho$. Furthermore, let $\{\Psi_k\}_{k=1}^{\infty}$ be an ONB of $\mathcal{F}^-$, such that $\Psi_k \in \mathcal{D}(\mathbb{H})$ for any $k \in \mathbb{N}$. Analogously to the boson case, we obtain

\[
\text{tr}_{\mathcal{F}^-}(\mathbb{H}^{\frac{1}{2}} \rho \mathbb{H}^{\frac{1}{2}}) = \sum_{k=1}^{\infty} \left( \mathbb{H}^{\frac{1}{2}} \rho \mathbb{H}^{\frac{1}{2}} \Psi_k \right)_{\mathcal{F}^-}.
\]

By Lemma 3.4, the positive semi-definite operator $\rho$ can be written as $\rho = \kappa \kappa^*$, where

\[
\kappa := \bigcup_{U} \left[ |\varphi_1 \wedge \ldots \wedge \varphi_n\rangle \langle \varphi_1 \wedge \ldots \wedge \varphi_n| \otimes [\text{tr}_{\mathcal{F}^-}(\Gamma(B))]^{-\frac{1}{2}} \Gamma(B^{\frac{1}{2}}) \right]
\]

with a decomposition $h = h_{\Psi} \otimes h_{\Phi} = n = \text{dim}(h_{\Psi}) < \infty$, an ONB $\{\psi_k\}_{k=1}^{n}$ of $h_{\Psi}$, a unitarily implementable Bogoliubov transformation $U$, and a positive semi-definite trace class operator $B \in \mathcal{B}(h_{\Phi})$. Hence,

\[
\omega(\mathbb{H}) = \sum_{k=1}^{\infty} \left\| \kappa^* \mathbb{H}^{\frac{1}{2}} \Psi_k \right\|^2_{\mathcal{F}^-}.
\]
Instead of a resolution of the identity by coherent states for bosons, we use the resolution of the identity by Slater determinants,

\[ 1_F = \lim_{N \to \infty} \lim_{M \to \infty} \sum_{l=0}^{N} \sum_{1 \leq i_1 < \ldots < i_l \leq M} |\varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l}|, \]

as in the proof of Lemma 3.6, in particular, Eq. (24). Then, we obtain

\[ \omega(\mathbb{H}) = \sum_{k=1}^{\infty} \lim_{N \to \infty} \lim_{M \to \infty} \sum_{l=0}^{N} \sum_{1 \leq i_1 < \ldots < i_l \leq M} \left| \left( \mathbb{H}^\dagger \psi_k, \kappa \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right) \right)_F \right|^2. \]

Because the sequence \( \left( k \mapsto \lim_{N \to \infty} \lim_{M \to \infty} \sum_{l=0}^{N} \sum_{1 \leq i_1 < \ldots < i_l \leq M} \left| \left( \mathbb{H}^\dagger \psi_k, \kappa \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right) \right)_F \right|^2 \right)_{N=1}^{\infty} \) is monotonously increasing, the monotone convergence theorem allows for an exchange of the \( k \)-summation and the first limit. Using the monotone convergence theorem a second time to exchange the second limit and the \( k \)-summation, we obtain

\[ \omega(\mathbb{H}) = \lim_{N \to \infty} \lim_{M \to \infty} \sum_{k=1}^{\infty} \sum_{l=0}^{N} \sum_{1 \leq i_1 < \ldots < i_l \leq M} \left| \left( \mathbb{H}^\dagger \psi_k, \kappa \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right) \right)_F \right|^2. \]

Furthermore, we change the order of the summations, since the sum is absolutely convergent, and get

\[ \omega(\mathbb{H}) = \lim_{N \to \infty} \lim_{M \to \infty} \sum_{l=0}^{N} \sum_{1 \leq i_1 < \ldots < i_l \leq M} \left| \kappa \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right), \mathbb{H} \kappa \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right) \right|_F. \]

Every vector \( \kappa \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right) \) defines a pure quasifree state, cf. the proof of Lemma 3.6. Since \( \langle \Psi, \mathbb{H}^\dagger \Psi \rangle_F \geq E^\text{pure}_{\text{BHF}} \) for any pure quasifree state \( |\Psi\rangle \langle \Psi|, \Psi \in F^- \), we finally have

\[ \omega(\mathbb{H}) \geq E^\text{pure}_{\text{BHF}} \lim_{N \to \infty} \lim_{M \to \infty} \sum_{l=0}^{N} \sum_{1 \leq i_1 < \ldots < i_l \leq M} \left| \rho \left( \varphi_{i_1} \wedge \ldots \wedge \varphi_{i_l} \right) \right|_F = E^\text{pure}_{\text{BHF}}. \]

This proves the assertion. \( \square \)

IV. PURE QUASIFREE STATES AND THEIR GENERALIZED ONE-PARTICLE DENSITY MATRIX

For a given generalized fermion 1-pdm \( \widetilde{\gamma} \), it is known that there is a pure quasifree state \( \omega \) which has \( \widetilde{\gamma} \) as its generalized 1-pdm, if and only if the generalized 1-pdm is a projection, i.e., \( \widetilde{\gamma}^2 = \widetilde{\gamma} \). For bosons, a similar statement is also known. In this section, we show that an even stronger relation holds:

**Theorem 4.1.** Let \( \omega \in \mathcal{Z}_\text{cen}^+ \) or \( \omega \in \mathcal{Z}^- \). The following statements are equivalent:

(i) \( \omega \) is a pure quasifree state.

(ii) The corresponding generalized 1-pdm \( \widetilde{\gamma} \) satisfies \( \text{tr}_0(\gamma) < \infty \) and

\[ \mathcal{S} \mathcal{S} = -\widetilde{\gamma} \quad \text{for bosons}, \quad \widetilde{\gamma}^2 = \widetilde{\gamma} \quad \text{for fermions}. \]

Recall \( \mathcal{S} = \frac{1}{2} h \oplus (-\frac{1}{2}) h \in B(h \oplus h) \). Note that, for bosons, we assume \( \omega \) to be centered and, thus, (i) is equivalent to the condition that \( \omega \) fulfills Wick's theorem. A proof of Theorem 4.1 in the fermion case is given in Subsection IV A. In Subsection IV B, we sketch the proof for bosons and discuss two consequences of this theorem afterwards.
A. Fermions

The theorem follows from the subsequent lemmas. The implication (i) \( \Rightarrow \) (ii) of Theorem 4.1 for fermions is given by the second assertion of Lemma 4.2 and the reverse by Lemma 4.3.

**Lemma 4.2.** If an operator \( \tilde{\gamma} = \begin{pmatrix} \nu & a \\ a^* & \tilde{\nu} \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h} \rightarrow \mathfrak{h} \oplus \mathfrak{h} \) satisfies \( 0 \leq \tilde{\gamma} \leq 1_{\mathfrak{h}} \), \( \text{tr}_h(\nu) < \infty \), and \( \tilde{\gamma}^2 = \tilde{\gamma} \), then there is a unique pure quasifree state \( \omega \in \mathcal{Z}^- \) that has \( \tilde{\gamma} \) as its generalized one-particle density matrix.

Furthermore, let \( \omega \in \mathcal{Z}^- \) be a pure quasifree state. Then, the corresponding generalized 1-pdm \( \tilde{\gamma} \) fulfills \( \tilde{\gamma}^2 = \tilde{\gamma} \).

This lemma is a consequence of Theorems 2.3 and 2.6 in Ref. 5. There is even a one-to-one relation between pure quasifree states and generalized 1-pdm’s fulfilling \( \tilde{\gamma}^2 = \tilde{\gamma} \).

**Lemma 4.3.** Let \( \omega \in \mathcal{Z}^- \). If the generalized 1-pdm \( \tilde{\gamma} \) corresponding to the state \( \omega \) satisfies \( \tilde{\gamma}^2 = \tilde{\gamma} \), then \( \omega \) is a pure quasifree state.

The proof is a modification of the proof of Theorem 10.4 in Ref. 18 (see also Theorem 2.6 in Ref. 5), where it is presupposed that \( \omega \) is quasifree.

**Proof.** Let \( \tilde{\gamma} = \begin{pmatrix} \nu & a \\ a^* & \tilde{\nu} \end{pmatrix} \) be the generalized 1-pdm of \( \omega \). There is an ONB \( \{ \phi_j \}_{j=1}^{\infty} \) of the one-particle Hilbert space of eigenvectors of \( \nu \) with associated eigenvalues \( \{ \lambda_i \}_{i=1}^{\infty} \), such that, for some \( K \in \mathbb{N}, \lambda_j = 1 \) if and only if \( j < K \). We define \( (1_{\mathfrak{h}} - \nu)^{-1/2} P_{\perp} \) := \( \sum_{j \geq K} (1 - \lambda_j)^{-1/2} |\phi_j\rangle \langle \phi_j| \) and \( \tilde{P} := \sum_{j < K} |\phi_j\rangle \langle \phi_j| \). The operator \( U = \left( \begin{array}{cc} U & 0 \\ 0 & U \end{array} \right) \) on \( \mathfrak{h} \oplus \mathfrak{h} \) with
\[
\begin{align*}
  u := (1_{\mathfrak{h}} - \nu)^{\frac{1}{2}}
  \quad \text{and} \quad
  v := \alpha (1_{\mathfrak{h}} - \tilde{\nu})^{-\frac{1}{2}} \tilde{P} + \tilde{P}
\end{align*}
\]
is a fermion Bogoliubov transformation and has a unitary representation which we denote by \( U \). We define the state \( \omega_U \in \mathcal{Z}^- \) by \( \omega_U(A) := \omega(U A \, U^*) \) for any \( A \in \mathcal{A}^- \). The corresponding generalized 1-pdm is \( \tilde{\gamma}_U = \begin{pmatrix} 0 & 0 \\ 0 & 1_{\mathfrak{h}} \end{pmatrix} \) and, by Lemma 2.14, \( \tilde{\gamma}_U = U^{*} \tilde{\gamma} U \). Consequently, \( \gamma_U = 0 \) and \( \gamma_U \) is a projection. Hence, for any \( A \in \mathcal{A}^- \), \( \omega_U(A) = \langle \Omega, A \, \Omega \rangle_{\mathcal{F}^+} \). Since \( U \) is a Bogoliubov transformation with unitary implementation \( U \) and invertible, we obtain for any \( A \in \mathcal{A}^- \)
\[
\omega(A) = \omega_U \left( U^* A \, U \right) = \langle \Omega, A \, \Omega \rangle_{\mathcal{F}^+}.
\]
Therefore, the state \( \omega \) is pure and quasifree which yields the assertion. \( \square \)

B. Bosons

Theorem 4.1 for bosons is a consequence of the following Lemmas 4.4 and 4.8.

**Lemma 4.4.** If an operator \( \nu = \begin{pmatrix} \nu & a \\ a^* & \tilde{\nu} \end{pmatrix} : \mathfrak{h} \oplus \mathfrak{h} \rightarrow \mathfrak{h} \oplus \mathfrak{h} \) satisfies \( \nu \geq 0 \), \( \text{tr}_h(\nu) < \infty \), and
\[
\nu S \nu = -\nu,
\]
then there is a centered pure quasifree state \( \omega \in \mathcal{Z}_{\text{pqf}}^+ \cap \mathcal{Z}_{\text{cen}}^+ \) that has \( \nu \) as its generalized one-particle density matrix. Furthermore, let \( \omega \in \mathcal{Z}_{\text{pqf}}^+ \cap \mathcal{Z}_{\text{cen}}^+ \) be a centered pure quasifree state. Then, the corresponding generalized 1-pdm \( \tilde{\gamma} \) fulfills (25).
For a proof, see, e.g., Refs. 15 and 18. Equation (25) is rewritten in a single equation for operators on \( \mathfrak{h} \), i.e., we do not need the matrices \( \gamma \) and \( S \).

**Proposition 4.5.** Let \( \omega \in Z^+ \) be a state with the generalized 1-pdm \( \gamma \) = \( \begin{pmatrix} \gamma_{22} & \gamma_{21} \\ \gamma_{12} & \gamma_{11} \end{pmatrix} \). Then

\[
\gamma S \gamma = -\gamma \Rightarrow \gamma^2 + \gamma = \alpha \alpha^*.
\]

**Proof.** The left statement is equivalent to the system of four equations

\[
\gamma^2 + \gamma = \alpha \alpha^*, \quad \bar{\gamma}^2 + \bar{\gamma} = \alpha^* \alpha, \quad \gamma \alpha = \alpha \bar{\gamma}, \quad \alpha^* \gamma = \bar{\gamma} \alpha^*.
\]

Hence, the implication \( \Rightarrow \) is immediate. It remains to prove \( \Leftarrow \), i.e., \( \gamma^2 + \gamma = \alpha \alpha^* \) implies the four equations above. Among those four equations, the first two equations are conjugate of each other and the last two equations are adjoint of each other. Thus, it is sufficient to show that \( \gamma^2 + \gamma = \alpha \alpha^* \) implies \( \gamma \alpha = \alpha \bar{\gamma} \). Assume that \( \gamma^2 + \gamma = \alpha \alpha^* \) holds. The map \( f(x) := \frac{\sqrt{1 + x}}{1/2} \) is the inverse of \( x \mapsto x + x^2, \mathbb{R}^+ \rightarrow \mathbb{R}^+ \). Then \( \gamma = f(\alpha \alpha^*) \) and \( \bar{\gamma} = f(\alpha^* \alpha) \). We approximate the function \( f \) by a sequence \( (p_n)_{n=1}^{\infty} \) of polynomials, uniformly on the compact interval \([0, \|\alpha \alpha^*\|_\infty]\).

Using \( (\alpha \alpha^*)^m \alpha = (\alpha \alpha^*)^m \), for any \( m \in \mathbb{N} \) and limits in operator norm, we obtain

\[
\gamma \alpha = f(\alpha \alpha^*) \alpha = \lim_{n \rightarrow \infty} p_n (\alpha \alpha^*) \alpha = \lim_{n \rightarrow \infty} \alpha p_n (\alpha^* \alpha) = \alpha f(\alpha^* \alpha) = \alpha \bar{\gamma},
\]

which proves the assertion.

**Remark 4.6.** In Ref. 3,

\[
\gamma = \frac{1}{2} (\cosh(2r) - 1) \quad \text{and} \quad \hat{\alpha} = \frac{1}{2} \sinh(2r)
\]

are used, where \( \{f, \alpha \bar{\gamma} \} \mathfrak{h} = \{f, \alpha g \} \mathfrak{h} \) and \( r : \mathfrak{h} \rightarrow \mathfrak{h} \) is an antilinear operator. \( r \) obeys \( \{f, r g\} \mathfrak{h} = \{g, r f\} \mathfrak{h} \) for any \( f, g \in \mathfrak{h} \) and \( r^2 \) is trace class. These two equations are, however, implied by \( \gamma^2 + \gamma = \alpha \alpha^* \) and, in turn, yield \( \gamma \alpha = \alpha \bar{\gamma} \).

Centered pure quasifree states can be characterized by a Bogoliubov transformation (see Ref. 15 for a proof):

**Lemma 4.7.** A centered boson state \( \omega \in Z^+_{cen} \) is pure quasifree if and only if there is a boson Bogoliubov transformation \( U : \mathfrak{h} \oplus \mathfrak{h} \rightarrow \mathfrak{h} \oplus \mathfrak{h} \) with unitary representation \( \mathbb{U}_U : \mathcal{F}^+ \rightarrow \mathcal{F}^+ \), such that \( \omega(A) = \langle \mathbb{U} \Lambda, A \mathbb{U} \Lambda \rangle_{\mathcal{F}^+} \) for any \( A \in \mathbb{A}^+ \).

The relation between a generalized 1-pdm fulfilling (25) and the corresponding centered pure quasifree state is even closer.

**Lemma 4.8.** Let \( \omega \in Z^+_{cen} \) and assume that the corresponding generalized 1-pdm \( \gamma \) = \( \begin{pmatrix} \gamma_{22} & \gamma_{21} \\ \gamma_{12} & \gamma_{11} \end{pmatrix} \) satisfies \( \gamma S \gamma = -\gamma \). Then, \( \omega \) is a centered pure quasifree state.

Since the proof is somewhat similar to the proof of Theorem 10.4 in Ref. 18, we only give the main steps. First, we define the boson Bogoliubov transformation \( U := (u \quad v) \), where \( u := (1 + \gamma)^{1/2} \) and \( v := \alpha (1 + \gamma)^{-1/2} \) are operators on \( \mathfrak{h} \). This Bogoliubov transformation has a unitary representation \( \mathbb{U} \). Next, we define a state \( \omega_U \in Z^+ \) by \( \omega_U(A) := \omega(\mathbb{U} \underline{A} \mathbb{U}^*) \). Finally, since \( \gamma_U = \begin{pmatrix} 0 & 0 \\ 0 & \gamma \end{pmatrix} \) is the generalized 1-pdm of \( \omega_U \) and, in particular, \( \gamma_U = 0 \), \( \omega_U \) is the vacuum state and \( \omega(A) = \langle \mathbb{U} \Lambda, A \mathbb{U} \Lambda \rangle_{\mathcal{F}^+} \).
A consequence of Lemma 4.8 is the following proposition.

**Proposition 4.9.** Let \( \omega \in \mathbb{Z}^+ \) be a state and

\[
\hat{\gamma} = \begin{pmatrix} \gamma & \alpha & b \\ \alpha^* & 1_b + \overline{\gamma} & \overline{b} \\ b^* & \overline{b}^* & 1 \end{pmatrix}
\]

the corresponding further generalized 1-pdm with \( \gamma : \mathfrak{h} \to \mathfrak{h} \) and \( \alpha^* : \mathfrak{h} \to \mathfrak{h} \) as defined in Eqs. (13) and (14), respectively. As in (19), the first moment \( b \in \mathfrak{h} \) of the state \( \omega \) is given by \( (f, b)_\mathfrak{h} := \omega(a(f)) \) for any \( f \in \mathfrak{h} \). If

\[
\hat{\gamma} Q_b \hat{\gamma} = -\hat{\gamma} \quad \text{with} \quad Q_b := \begin{pmatrix} 1_b & 0 & -b \\ 0 & -1_b & \overline{b} \\ -b^* & \overline{b}^* & -1 \end{pmatrix},
\]

then \( \omega \) is a pure quasifree state.

Note that \( Q_b \) is a self-adjoint operator on \( \mathcal{H}_{\text{gen}} := \mathfrak{h} \oplus \mathfrak{h} \oplus \mathbb{C} \).

**Proof.** If \( \omega \) is centered, we have \( b = 0 \) and (26) reduces to \( \hat{\gamma} Q_b \hat{\gamma} = -\hat{\gamma} \) which is equivalent to \( \hat{\gamma} \tilde{S} \hat{\gamma} = -\hat{\gamma} \). So, Lemma 4.8 directly yields the assertion. Now, we do not assume the state to be centered. Then, for the Weyl transformation \( \mathbb{W}_b : \mathcal{F}^+ \to \mathcal{F}^+ \), we define the state \( \omega_0 \in \mathbb{Z}^+ \) by \( \omega_0(A) := \omega(\mathbb{W}_b^* A \mathbb{W}_b) \) for any \( A \in \mathcal{A}^+ \). First, we show that \( b_0 = 0, g_0 = \gamma - |b\rangle \langle b|, \) and \( \alpha_0^* = \alpha^* - |\overline{b}\rangle \langle \overline{b}| \) for this state \( \omega_0 \). For any \( f \in \mathfrak{h} \), we have

\[
(b_0, f)_\mathfrak{h} := \omega_0(a^*(f)) = \omega(a^*(f) - (b, f)_\mathfrak{h} \mathbb{1}_F) = (b, f)_\mathfrak{h} - (b, f)_\mathfrak{h} = 0.
\]

Thus, \( b_0 = 0 \) and \( \omega_0 \) is a centered state. Furthermore, for any \( f, g \in \mathfrak{h} \),

\[
(f, \gamma_0 g)_\mathfrak{h} = \omega([a^*(g) - (b, g)_\mathfrak{h} \mathbb{1}_F][a(f) - (f, b)_\mathfrak{h} \mathbb{1}_F]) = (f, \gamma_0 g)_\mathfrak{h} - (f, b)_\mathfrak{h} (b, g)_\mathfrak{h}.
\]

An analogous calculation yields \( [f, \alpha_0^* g]_\mathfrak{h} = \omega(a^*(g)a^*(f)) - (b, g)_\mathfrak{h} (b, f)_\mathfrak{h} \). Next, we consider (26). We decompose the operator \( Q_b \) as \( Q_b = R_b \tilde{S} R_b^\dagger \), where the operators \( R_b, \tilde{S} : \mathcal{H}_{\text{gen}} \to \mathcal{H}_{\text{gen}} \) are given by

\[
R_b := \begin{pmatrix} -1_b & 0 & 0 \\ 0 & -1_b & 0 \\ b^* & \overline{b} & 1 \end{pmatrix} \quad \text{and} \quad \tilde{S} := \begin{pmatrix} 1_b & 0 & 0 \\ 0 & -1_b & 0 \\ 0 & 0 & -1 \end{pmatrix}.
\]

Since \( R_b \) is invertible, (26) is equivalent to

\[
(R_b^\dagger \hat{\gamma} R_b) \tilde{S} (R_b^\dagger \hat{\gamma} R_b) = -R_b^\dagger \hat{\gamma} R_b.
\]

(26')

A straightforward computation yields

\[
R_b^\dagger \hat{\gamma} R_b = \begin{pmatrix} \gamma - |b\rangle \langle b| & \alpha - |b\rangle \langle \overline{b}| & 0 \\ \alpha^* - |\overline{b}\rangle \langle b| & 1_b + \overline{\gamma} - |\overline{b}\rangle \langle \overline{b}| & 0 \\ 0 & 0 & 1 \end{pmatrix}.
\]

Summarizing the results, we obtain \( R_b^\dagger \hat{\gamma} R_b = \begin{pmatrix} \gamma_0 & \alpha_0 & 0 \\ \alpha_0^* & 1_b + \overline{\gamma}_0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \), which is the further generalized 1-pdm \( \tilde{\gamma}_0 \) of the state \( \omega_0 \). Thus, (26) implies \( \tilde{\gamma}_0 \tilde{S} \tilde{\gamma}_0 = -\tilde{\gamma}_0 \). Since the upper left \( 2 \times 2 \)-matrix of \( \tilde{\gamma}_0 \) (which is an operator on \( \mathfrak{h} \oplus \mathfrak{h} \)) is the generalized 1-pdm \( \tilde{\gamma}_0 \) and \( \tilde{S} \) is diagonal, we find \( \tilde{\gamma}_0 \tilde{S} \tilde{\gamma}_0 = -\tilde{\gamma}_0 \). Hence, the requirements of Theorem 4.8 are satisfied for the state \( \omega_0 \). Therefore, \( \omega_0 \) is a pure quasifree state. So, by Remark 2.9, \( \omega \) is also pure and quasifree.
An important set of states which are related to the vacuum state via a Weyl transformation is the set of coherent states. Recall that a state $\omega \in \mathbb{Z}^+$ is called coherent if there is an $f \in \mathfrak{h}$ and a Weyl transformation $\mathbb{W}_f : \mathcal{F}^+ \rightarrow \mathcal{F}^+$, such that, for any $A \in \mathcal{A}^+$,

$$\omega(A) = \langle \mathbb{W}_f \Omega, A \mathbb{W}_f^* \Omega \rangle_{\mathcal{F}^+}.$$  

Corollary 4.10. Equation (26) is satisfied for every coherent state.

Proof. For every coherent state $\omega$, we can find $\phi \in \mathfrak{h}$, such that

$$\omega(A) = \langle \Omega, \mathbb{W}_\phi A \mathbb{W}_\phi^* \Omega \rangle_{\mathcal{F}^+},$$

where $\mathbb{W}_\phi : \mathcal{F}^+ \rightarrow \mathcal{F}^+$ is a Weyl transformation. We have $b = \phi$, because, for any $f \in \mathfrak{h}$,

$$(b, f)_b = \langle \Omega, \mathbb{W}_\phi a^*(f) \mathbb{W}_\phi^* \Omega \rangle_{\mathcal{F}^+} = \langle \Omega, [a^*(f) + (\phi, f)_b 1_{\mathcal{F}^+}] \Omega \rangle_{\mathcal{F}^+},$$

where we use $(\Omega, a^*(f) \Omega)_{\mathcal{F}^+} = \langle a(f) \Omega, \Omega \rangle_{\mathcal{F}^+} = 0$. For the 1-pdm $\gamma$, we find

$$(f, \gamma g)_b = \langle \Omega, [a^*(g) + (b, g)_b 1_{\mathcal{F}^+}][a(f) + (f, b)_b 1_{\mathcal{F}^+}] \Omega \rangle_{\mathcal{F}^+} = (f, b)_b (b, g)_b,$$

for every $f, g \in \mathfrak{h}$, using $\phi = b$. Thus, $\gamma = |b\rangle \langle b|$. Furthermore, $a^* = |b\rangle \langle b|$ by an analogous calculation. Finally, we obtain $\mathcal{R}_\gamma^+ \mathcal{R}_\phi = 0_b \otimes 1_b \otimes 1$, which obviously fulfills (26). \qed

APPENDIX: BOSONIC REPRESENTABILITY CONDITIONS AND THE GENERALIZED TWO-PARTICLE DENSITY MATRIX

1. Particle number-conserving systems

To our knowledge, sets of representability conditions given in the literature are for particle number-conserving systems for fermions, as well as for bosons. That is, only states, that fulfill

$$\omega\left(\prod_{k=1}^n a^*(f_k) \prod_{l=1}^m a(g_l)\right) = 0$$

for any two sets $\{f_k\}_{k=1}^n, \{g_l\}_{l=1}^m \subseteq \mathfrak{h}$ with $m, n \in \mathbb{N} \cup \{0\}$ and $m \neq n$, are considered. Since the dynamics of many realistic physical boson systems do not conserve the particle number, an alternative should be found. First, we restate some representability conditions for bosons.

Definition A.1. Let $(\gamma, \Gamma)$ be a pair of operators on $\mathfrak{h}$ and $\mathfrak{h} \otimes \mathfrak{h}$, respectively. We say that $(\gamma, \Gamma)$ satisfies the representability conditions up to second order with particle number-conservation if

1. $(\gamma, \Gamma)$ is admissible,
2. $\Gamma$ satisfies the P-condition, i.e., $\Gamma \geq 0$, and
3. the G-condition, i.e., for any $A \in \mathcal{B}(\mathfrak{h})$ we have

$$\text{tr}_{\mathfrak{h} \otimes \mathfrak{h}}((A^* \otimes A) [\Gamma + \text{Ex}(\gamma \otimes 1_{\mathfrak{h}})]) \geq \left|\text{tr}_{\mathfrak{h}} (A \gamma)\right|^2.$$  

These conditions can be found, e.g., in Refs. 12 and 13. Note that these conditions are only necessary conditions, but do not ensure that the considered operators are one- and two-particle density matrices. Furthermore, we omit here other known conditions like the $T_1$- and $T_2$-condition, cf. Ref. 11.

Remark A.2. The Q-condition is omitted since it follows from the P-condition and the positivity of $\gamma$, see Ref. 13. Nevertheless, in the same manner, we can rephrase the Q-condition from Ref. 13 as $\Gamma \geq - (\delta_{\mathfrak{h} \otimes \mathfrak{h}} + \text{Ex}) (\gamma \otimes 1_{\mathfrak{h}} + 1_{\mathfrak{h}} \otimes \gamma + 1_{\mathfrak{h}} \otimes 1_{\mathfrak{h}})$.

The representability conditions for bosons up to second order can be derived in the same spirit as it is done for fermions in Ref. 4.

Theorem A.3. Let $\omega$ be a linear continuous functional on $\mathcal{A}^+$ such that $\omega(1_{\mathcal{F}^+}) = 1$, $\omega(\mathbb{N}_2) < \infty$, and $\omega(a^n(f_1) \ldots a^{2n-1}(f_{2N-1})) = 0$ for all $N \in \mathbb{N}$, where $a^n(f_k)$ denotes either a creation or...
annihilation operator. Furthermore, let $\Gamma_\omega$ and $\gamma_\omega$ be the corresponding 1- and 2-pdm and $\{\varphi_k\}_{k=1}^\infty$ an ONB of $\mathfrak{h}$. Then the following statements are equivalent:

(i) For any polynomial $P_r \in \mathcal{A}^+$ in creation and annihilation operators of degree $r \leq 2$, we have $\omega(P_r P_r^*) \geq 0$.

(ii) $\gamma_\omega \geq 0$ and $\Gamma_\omega$ fulfills the G- and P-conditions.

Since the proof is analogous to the fermion case considered in Ref. 4, we omit the details here. Note that, unlike the fermion case, the trace class conditions on the 1- and 2-pdm cannot be derived from the polynomials since the boson creation and annihilation operators are unbounded.

2. Systems without particle number-conservation and the generalized two-particle density matrix

We generalize the definition of the representability conditions up to second order to systems—and, thus, states—which do not conserve the particle number. These representability conditions arise in the same manner as those for particle conserving states by considering expectation values of polynomials up to second order in the creation and annihilation operators. Due to the absence of particle number-conservation, the expectation values of terms, in which the number of creation operators is not equal to the number of annihilation operators, do, in general, not vanish. A simple consequence of Definition 2.22 is the following proposition.

Proposition A.4. The representability conditions up to second order are satisfied if the pair $(\gamma$, $\Gamma)$ of operators on $\mathfrak{h}$ and $\mathfrak{h} \otimes \mathfrak{h}$ is admissible and $\hat{\Gamma}$ is positive semi-definite as an operator on $\mathfrak{g}_{\text{sim}}$.

Let $\omega$ be a linear functional on the operators on $\mathcal{F}^+$. Since, on the one hand, any polynomial up to second order in creation and annihilation operators can be written as $P = P_2(F) + P_1(f) + \nu$ with $F \in \bigoplus^4 \mathfrak{h}^\otimes 2$, $f \in \bigoplus^3 \mathfrak{h}$, $\nu \in \mathbb{C}$, Definition 2.22 yields

$$\omega(P P^*) = \left\langle \left( \begin{array}{c} F \\ f \\ \nu \end{array} \right), \hat{\Gamma} \left( \begin{array}{c} F \\ f \\ \nu \end{array} \right) \right\rangle_{\mathfrak{g}_{\text{sim}}}.$$ 

On the other hand, every element of $\mathfrak{g}_{\text{sim}}$ can be written as a vector with $F \in \bigoplus^4 \mathfrak{h}^\otimes 2$, $f \in \bigoplus^3 \mathfrak{h}$, $\nu \in \mathbb{C}$. Thus, the representability conditions up to second order are exactly those arising from

$$\omega(P P^*) \geq 0$$

for any polynomial $P$ in creation and annihilation operators of degree $r \leq 2$.

Remark A.5. Since the generalized 1-pdm appears as a block in the generalized 2-pdm, it inherits the definiteness property from the generalized 2-pdm.

If one varies only over particle number-conserving states, then $\hat{\Gamma}$ assumes a block-diagonal form and the complexity of the representability reduces considerably. In fact, only three independent conditions remain which are reminiscent of the G- and P-conditions in quantum chemistry (see Theorem A.3).


