



The time-dependent Hartree–Fock–Bogoliubov equations for Bosons

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Abstract. We introduce the map of dynamics of quantum Bose gases into dynamics of quasifree states, which we call the “nonlinear quasifree approximation”. We use this map to derive the time-dependent Hartree–Fock–Bogoliubov (HFB) equations describing the dynamics of quantum fluctuations around a Bose–Einstein condensate. We prove global well-posedness of the HFB equations for pair potentials satisfying suitable regularity conditions, and we establish important conservation laws. We show that the space of solutions of the HFB equations has a symplectic structure reminiscent of a Hamiltonian system. This is then used to relate the HFB equations to the HFB eigenvalue equations discussed in the physics literature. We also construct Gibbs equilibrium states at positive temperature associated with the HFB equations, and we establish criteria for the appearance of Bose–Einstein condensation.

1. Introduction

In this paper, we derive the time-dependent *Hartree–Fock–Bogoliubov (HFB) equations* describing quantum fluctuations of a non-relativistic Bose gas around a Bose–Einstein condensate and study their properties.

1.1. Quantum many-body problem

The starting point of our analysis is a second-quantized description of a quantum-mechanical many-body system of Bose point particles (bosonic atoms). We first consider systems of finitely many particles. The Hilbert space of pure state vectors is given by the bosonic Fock space:

$$\mathcal{F} := \bigoplus_{n=0}^{\infty} \mathcal{F}^{(n)}, \quad (1)$$

where $\mathcal{F}^{(n)} := \mathfrak{h}^{\otimes_{\text{sym}} n}$, for $n \geq 1$, is the n -fold symmetric tensor product of the one-particle Hilbert space

$$\mathfrak{h} := L^2(\mathbb{R}^d),$$

accounting for the Bose–Einstein statistics of the particles, and $\mathcal{F}^{(0)} := \mathbb{C} \cdot \Omega$ is the one-dimensional vacuum sector spanned by the normalized vacuum vector Ω .

Building blocks of operator calculus on $\mathcal{F}$ are annihilation and creation operator-valued distributions $\psi(f)$ and $\psi^*(f)$, $f \in \mathfrak{h}$, which are adjoints of each other and satisfy the canonical commutation relations (CCR):

$$[\psi(f_1), \psi^*(f_2)] = \langle f_1 | f_2 \rangle_{\mathfrak{h}}, \quad [\psi(f_1), \psi(f_2)] = [\psi^*(f_1), \psi^*(f_2)] = 0, \quad (2)$$

and $\psi(f_1)\Omega = 0$, for all $f_1, f_2 \in \mathfrak{h}$, see, e.g., [13]. We will write $\psi^\sharp(x)$ for their formal distribution kernels $\psi^*(x)$ and $\psi(x)$, i.e., $\psi^*(f) = \int f(x) \psi^*(x) dx$, $\psi(f) = \int \overline{f(x)} \psi(x) dx$, and the CCR read

$$[\psi(x), \psi^*(y)] = \delta(x - y), \quad [\psi(x), \psi(y)] = [\psi^*(x), \psi^*(y)] = 0. \quad (3)$$

The time evolution of the system is generated by the quantum Hamiltonian:

$$\mathbb{H} = \int d \psi^*(x) h \psi(x) + \frac{1}{2} \int dx dy v(x - y) \psi^*(x) \psi^*(y) \psi(x) \psi(y), \quad (4)$$

where, in the position-space representation, the operator h is given by

$$h := -\Delta + V(x), \quad x \in \mathbb{R}^d, \quad d = 1, 2, 3, \dots,$$

with Δ the Laplacian acting on $\mathfrak{h}$.

We always impose the following conditions:

$$(a) \quad \text{The external potential } V \text{ is infinitesimally bounded} \\ \text{with respect to the Laplacian } -\Delta. \quad (5)$$

$$(b) \quad \text{The pair potential } v \text{ is even, } v(x) = v(-x), \\ \text{and relatively bounded with respect to } \Delta. \quad (6)$$

These conditions imply that $\mathbb{H}$ is self-adjoint on the domain of the operator

$$\mathbb{H}_0 := \int dx \psi^*(x)(-\Delta)\psi(x) \quad (7)$$

(see Appendix A). We note that these conditions allow both V and v to have Coulomb singularities.

Let $W^{p,r}(\mathbb{R}^d)$ denote the standard Sobolev space over $\mathbb{R}^d$. In Sect. 4, we will use a stronger condition on v :

$$(b') \quad \text{The pair potential } v \text{ is even, } v(x) = v(-x), \\ \text{and satisfies } v \in W^{p,1}, \text{ for some } p > d. \quad (8)$$

States of the system are normalized positive linear ('expectation') functionals, ω , on the Weyl algebra $\mathfrak{W}$ over Schwartz space $\mathcal{S}(\mathbb{R}^d)$, which is generated by Weyl operators,

$$W(f) := e^{i\phi(f)}, \quad \text{with } \phi(f) := \psi^*(f) + \psi(f),$$

(see [13], Section 5.2.3). The set of states ω is denoted by $\mathfrak{S}$, and $\mathcal{S}(\mathbb{R}^d) \ni f \mapsto \omega[W(f)] \in \mathbb{C}$ can be viewed as its infinite-dimensional Fourier transform or characteristic function, i.e., the generating functional of all correlations functions, see below.

States correspond either to a finite number of Bose particles, as in the case of BEC experiments in traps, or to an infinitely extended gas at a nonzero particle density and some fixed temperature. States $\omega \in \mathfrak{S}$ of finitely many particles are given by density operators on Fock space $\mathcal{F}$, i.e., there exists a positive, trace-class operator D_ω on $\mathcal{F}$ of unit trace such that $\omega(\mathbb{A}) = \text{Tr}(\mathbb{A}D_\omega)$, for all bounded operators $\mathbb{A}$ on $\mathcal{F}$ (and in particular for all elements $\mathbb{A} \in \mathfrak{W}$).

It will be convenient to consider states defined on arbitrary products:

$$\psi^\sharp(f_1) \dots \psi^\sharp(f_n),$$

of creation- and annihilation operators. Expectations of such products in a state ω , henceforth called *correlation functions*, can be defined by applying partial derivatives, ∂_{s_k} , to expectation values

$$\omega(W(s_1 f_1) \dots W(s_n f_n))$$

of Weyl operators. We will only consider states with the property that these derivatives, and hence, the corresponding correlation functions, exist, for arbitrary n ; such states are called *regular states*. Of particular interest to us are correlation functions with $n \leq 4$. Their existence is guaranteed by assuming, e.g., that $\omega(\mathbb{N}^2) < \infty$, where $\mathbb{N}$ is the particle number operator, $\mathbb{N} := \int dx \ \psi^*(x)\psi(x)$. This assumption implies, in particular, that ω is given by a density operator on $\mathcal{F}$. (We remark, however, that existence of correlation functions follows from considerably weaker assumptions, e.g., from an appropriate version of the assumption that the particle density in the gas is finite.)

The multilinear functionals $\omega(\psi^\sharp(f_1) \dots \psi^\sharp(f_n))$, for $f_1, \dots, f_n \in \mathcal{S}(\mathbb{R}^d)$, are given by tempered distributions (this is the nuclear theorem), which we formally write as:

$$\omega(\psi^\sharp(x_1) \dots \psi^\sharp(x_n)).$$

By an “observable”, we refer either to an element of the Weyl algebra $\mathfrak{W}$ or to a linear combination of operators of the form $\psi^\sharp(f_1) \dots \psi^\sharp(f_n)$. (We remark that the term “observable” is, however, usually reserved for products $\psi^\sharp(f_1) \dots \psi^\sharp(f_n)$ that are gauge-invariant, i.e., invariant under phase transformations, $\psi \mapsto e^{i\theta}\psi$, $\psi^* \mapsto e^{-i\theta}\psi^*$.)

The time evolution of regular states is given by the von Neumann–Landau equation [29, 48] (see also [10, 43], and [26]) for some history)

$$i \partial_t \omega_t(\mathbb{A}) = \omega_t([\mathbb{A}, \mathbb{H}]), \quad (9)$$

for arbitrary observables $\mathbb{A}$, which extends the standard von Neumann–Landau equation to general C^* -algebras (see, e.g., [13, 35]).

1.2. Quasifree states and truncated expectations

Since the evolution Eq. (9) is extremely complicated to analyze, one is interested in manageable approximations to it. Our approximation consists of restricting the dynamics given by (9) to *quasifree states*, the simplest—yet sufficiently rich—class of states generalizing the Hartree and Hartree–Fock ones, on the one hand, and the Gaussian random processes, on the other, as has been first realized and used in [6].¹

Quasifree states are defined in terms of truncated expectations, which we define next. We use the short-hand notation $\psi_j := \psi^{\sharp_j}(x_j)$. The n^{th} order *truncated expectations* (*correlation functions*), $\omega^T(\psi_1, \dots, \psi_n)$, of a state ω are defined recursively through

$$\omega(\psi_1 \cdots \psi_n) = \sum_{P_n} \prod_{J \in P_n} \omega^T(\psi_{i_1}, \dots, \psi_{i_{|J|}}), \quad (10)$$

where the P_n are partitions of the ordered set $\{1, \dots, n\}$ into ordered subsets, J . The simplest examples of truncated (or connected) correlations are

$$\begin{aligned} \omega^T(\psi(x)) &= \omega(\psi(x)), \\ \omega^T(\psi_1, \psi_2) &= \omega(\psi_1 \psi_2) - \omega(\psi_1) \omega(\psi_2). \end{aligned} \quad (11)$$

A state ω is called *quasifree* if truncated n -point expectations vanish for $n > 2$, i.e.,

$$\omega^T(\psi_1, \dots, \psi_n) = 0, \quad \forall n > 2, \quad (12)$$

We denote quasifree states by ω^q and the set of quasifree states by $\mathfrak{Q} \subset \mathfrak{S}$.

It follows from the definition that all n -point expectations, $\omega^q(\psi_1^{\sharp_1} \cdots \psi_n^{\sharp_n})$, with $n > 2$, in a quasifree state ω^q can be expressed in terms of $\omega^q(\psi_i^{\sharp_i})$ and $\omega^q(\psi_j^{\sharp_j} \psi_k^{\sharp_k})$, with $i, j, k \in \{1, \dots, n\}$. The explicit formula is called Wick's formula, or *Wick's theorem*; see [13]. Examples for small orders are given in Appendix B.

Given an arbitrary, not necessarily quasifree state $\omega \in \mathfrak{S}$, with $\omega(\mathbb{N}) < \infty$, there exists a unique quasifree state, denoted $q[\omega] \in \mathfrak{Q}$, such that expectations

$$\omega(\psi_1^{\sharp_1}) = q[\omega](\psi_1^{\sharp_1}) \quad \text{and} \quad \omega(\psi_1^{\sharp_1} \psi_2^{\sharp_2}) = q[\omega](\psi_1^{\sharp_1} \psi_2^{\sharp_2}) \quad (13)$$

of quadratic or lower order agree (see Sect. 1.4). We call the state $q[\omega]$ the quasifree reduction of ω .² The map $q : \mathfrak{S} \rightarrow \mathfrak{Q}$ is idempotent, $q \circ q = q$, and acts as a projection of the convex space $\mathfrak{S}$ of all states onto the space of quasifree states $\mathfrak{Q}$.

1.3. Quasifree dynamics

As mentioned above, detailed properties of the dynamics of a many-body system described by the von Neumann–Landau equation (9) are difficult to unravel, and approximations are therefore needed to extract interesting qualitative features.

¹The notion of quasifree states was introduced in [45]; see [13] and references therein.

²This notion was introduced in [2] (see below). For a related notion in the context the gauge invariant twice differentiable states, see [41]. For the definition of the gauge invariant states, see Sect. 1.3 below.

The main idea is to restrict the dynamics to quasifree states. However, the property of being quasifree is not preserved by the dynamics given by (9), and the main question here is how to map the true quantum evolution onto the class of quasifree states.

The *effective* dynamics we propose replaces Eq. (9), with an initial condition $\omega_0 \in \mathfrak{S}$, by the equation

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]), \quad \text{with } \omega_{t=0}^q = q[\omega_0], \quad (14)$$

for all observables $\mathbb{A}$ that are at most *quadratic* in creation- and annihilation operators.

For the Hamiltonian $\mathbb{H}$ given by (4), the commutator $[\mathbb{A}, \mathbb{H}]$ contains products of at most four creation- and annihilation operators; their expectation in ω_t^q is then evaluated by using Wick's theorem for the quasifree state ω_t^q .

In contrast to the von Neumann–Landau equation (9), the *quasifree dynamics* (14) is *nonlinear*.

Of course, one expects the effective evolution to be close the original one only if ω_0 is close to $q[\omega_0]$ in an appropriate sense. We emphasize that, in general,

$$\omega_t^q \neq q[\omega_t],$$

even if the initial state $\omega_0 = q[\omega_0] \in \mathfrak{Q}$ is quasifree. That is, the trajectory of quasifree states ω_t^q determined by (14) is *not* the projection, q , of the trajectory ω_t of states evolving according to the full dynamics in (9) onto the space $\mathfrak{Q}$ of quasifree states.

We call (14) the *nonlinear quasifree approximation* (it was called the quasifree reduction in [3].)

The deviation of a state $\omega \in \mathfrak{S}$ from its quasifree reduction $q[\omega] \in \mathfrak{Q}$ can be quantified in terms of their relative entropy $S_{\text{rel}}(\omega, q[\omega]) := \text{Tr}\{D_\omega(\ln[D_\omega] - \ln[D_{q[\omega]}])\}$, provided ω and hence $q[\omega]$ are given by density operators D_ω and $D_{q[\omega]}$, respectively [20]. In fact, $S_{\text{rel}}(\omega, q[\omega])$ may be viewed as the distance of ω to $\mathfrak{Q}$, since $S_{\text{rel}}(\omega, \omega') \geq 0$ with equality if, and only if, $\omega = \omega'$ and

$$S_{\text{rel}}(\omega, q[\omega]) = \inf_{q \in \mathfrak{Q}} S_{\text{rel}}(\omega, q). \quad (15)$$

It has been shown in [7] that for pure states the quasifree dynamics as defined above ([3]) is a consequence of the Dirac–Frenkel principle, in which the right side of the von Neumann–Landau equation (9) is projected onto a selected class of states.

We will show that Eq. (14) is equivalent to the nonlinear, self-consistent evolution equation

$$i\partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}_{\text{hfb}}(\omega_t^q)]), \quad (16)$$

for all observables $\mathbb{A}$, where $\mathbb{H}_{\text{hfb}}(\omega^q)$ is an explicit *quadratic* Hamiltonian given in Eq. (44), which depends on a quasifree state ω^q ; see Theorem 2.3. The equivalence holds for observables linear or quadratic in creation- and annihilation operators.

Equation (14), with the Hamiltonian $\mathbb{H}$ given by (4), is equivalent to the HFB Eqs. (20)–(22) derived from it below.

A state $\omega \in \mathfrak{S}$ is called $U(1)$ -gauge invariant, if it satisfies

$$\omega(\psi_\theta^\sharp(x_1) \cdots \psi_\theta^\sharp(x_n)) = \omega(\psi^\sharp(x_1) \cdots \psi^\sharp(x_n)),$$

for all $\theta \in \mathbb{R}$ and all $x_1, \dots, x_n \in \mathbb{R}^3$, where $\psi_\theta(x) := e^{i\theta} \psi(x)$. A quasifree state ω^q is $U(1)$ -gauge invariant iff ϕ_{ω^q} and σ_{ω^q} are vanishing. Indeed, $\omega^q(\psi(x)) = \omega^q(\psi_\theta(x)) = e^{i\theta} \omega^q(\psi(x))$, for all θ , implies $\omega^q(\psi(x)) = 0$. A similar argument applies to $\omega^q(\psi(x)\psi(y))$. If the initial state ω_0^q is a $U(1)$ -gauge invariant quasifree state, $\mathbb{H}$ is given by (4), and ω_t^q is the solution of Eq. (14), then ω_t^q is also a $U(1)$ -gauge invariant quasifree state. Then, one can show that the self-consistent Eq. (16) and the HFB Eqs. (39)–(43), reduce to the bosonic Hartree–Fock equation, i.e., to the HFB equations with $\phi_t = 0$, $\sigma_t = 0$, and γ_t being the only dynamical quantity.

1.4. HFB equations for truncated expectations

As was mentioned above, a quasifree state $\omega^q \in \mathfrak{Q}$ determines, and is determined by, the truncated expectations up to second order in the following sense:

1. $\omega \rightarrow \Gamma$: Given a (not necessarily quasifree) state $\omega \in \mathfrak{S}$ and its expectations

$$\begin{cases} \phi(x) &:= \omega[\psi(x)], \\ \gamma(x; y) &:= \omega[\psi^*(y) \psi(x)] - \omega[\psi^*(y)] \omega[\psi(x)], \\ \sigma(x, y) &:= \omega[\psi(x) \psi(y)] - \omega[\psi(x)] \omega[\psi(y)], \end{cases} \quad (17)$$

up to second order, and denoting by γ and σ the operators with integral kernels given by $\gamma(x, y)$ and $\sigma(x, y)$, respectively, we have that (see (51) below)

$$\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \geq 0, \quad (18)$$

where $\bar{A} := C\sigma C$, with C denoting complex conjugation in the position-space representation, (i.e., complex conjugation of wave functions of spatial variables). Note in passing that this implies, in particular, that

$$\gamma = \gamma^* \geq 0 \text{ and } \sigma^* = \bar{\sigma}. \quad (19)$$

2. $\Gamma \rightarrow \omega^q$: Conversely, given $\gamma = \gamma^* \geq 0$ and $\sigma^* = \bar{\sigma}$ such that $\Gamma := \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \geq 0$ obeys (18) and $\phi \in L^2(\mathbb{R}^d)$, there exists a unique quasifree state $\omega^q \in \mathfrak{Q}$ such that (17) holds true with ω^q replacing ω .

Actually, the condition that $\phi \in L^2(\mathbb{R}^d)$ is too restrictive and can be relaxed, depending on the context.

3. $\omega \rightarrow q[\omega]$: Given a state $\omega \in \mathfrak{S}$ and going through 1. and 2. above yields the quasifree reduction $q[\omega] := \omega^q$ of ω .

The matrix operator in (18) is called “generalized one-particle density matrix”. The positivity condition on Γ in (18) can be expressed directly in terms of γ and σ ; see [4], [3]. The steps 1. and 2., whose composition yields the quasifree reduction q , were first carried out in [2, Lemmata 3.2–3.5].

We will use (18) in proving the global existence for the HFB equations (see Proposition 3.1(4) and the paragraph after Eq. (90)).

Evaluating (14) for monomials $\mathbb{A} \in \mathcal{A}^{(2)}$, where

$$\mathcal{A}^{(2)} := \{ \psi(x), \psi^*(x)\psi(y), \psi(x)\psi(y) \},$$

yields a system of coupled nonlinear PDE’s for $(\phi_t, \gamma_t, \sigma_t)$, the *Hartree–Fock–Bogoliubov (HFB) equations*,

$$i \partial_t \phi_t = (h + v * d(\gamma_t) + v \sharp \gamma_t) \phi_t + (v \sharp \sigma_t^{\phi_t}) \bar{\phi}_t, \quad (20)$$

$$i \partial_t \gamma_t = [h + v * d(\gamma_t^{\phi_t}) + v \sharp \gamma_t^{\phi_t}, \gamma_t] + (v \sharp \sigma_t^{\phi_t}) \sigma_t^* - \sigma_t (v \sharp \sigma_t^{\phi_t})^*, \quad (21)$$

$$i \partial_t \sigma_t = [h + v * d(\gamma_t^{\phi_t}) + v \sharp \gamma_t^{\phi_t}, \sigma_t]_+ + [v \sharp \sigma_t^{\phi_t}, \gamma_t]_+ + v \sharp \sigma_t^{\phi_t}, \quad (22)$$

where $[A_1, A_2]_+ = A_1 A_2^T + A_2 A_1^T$, $A^T := \overline{A^*}$, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$, $\sigma^\phi := \sigma + |\phi\rangle\langle\bar{\phi}|$. Moreover, $d(\alpha)(x) := \alpha(x, x)$, and $v * d(\gamma)$ is multiplication by the convolution of v with the one-particle density corresponding to γ , and the Schwartz integral kernel $v \sharp \alpha(x, y) := v(x, y) \alpha(x, y)$ results from the product of $v(x - y)$ with the integral kernel of α .

The HFB equations are presented again in Eqs. (39)–(43), below. Since quasifree states are characterized by their truncated expectations ϕ , γ and σ , this system of equations is equivalent to Eq. (14).

For comparison of the HFB Eqs. (39)–(43) with the physics literature, we formally assume the pair interaction potential v to be a delta distribution,

$$v(x - y) = g \delta(x - y), \quad (23)$$

where $g \geq 0$ is a coupling constant. The HFB Eqs. (20)–(22) then assume the simpler form:

$$i \partial_t \phi_t = h_{g\delta}(\gamma_t^{\phi_t}) \phi_t + g d(\sigma_t^{\phi_t}) \bar{\phi}_t - 2g |\phi_t|^2 \phi_t, \quad (24)$$

$$i \partial_t \gamma_t = [h_{g\delta}(\gamma_t^{\phi_t}), \gamma_t] + g d(\sigma_t^{\phi_t}) \sigma_t^* - g \sigma_t \overline{d(\sigma_t^{\phi_t})}, \quad (25)$$

$$i \partial_t \sigma_t = [h_{g\delta}(\gamma_t^{\phi_t}), \sigma_t]_+ + g [d(\sigma_t^{\phi_t}), \gamma_t]_+ + d(\sigma_t^{\phi_t}), \quad (26)$$

$$\text{where } h_{g\delta}(\gamma) := h + 2gd(\gamma), \text{ with } h \text{ as in 4.} \quad (27)$$

(Note that here and in what follows, we denote *multiplication operators* and *functions* by which they multiply by the *same symbols*. The meaning is always clear from context.) In our results (see Theorem 2.2) and proofs, we always assume that the two-body potential is smooth.

The physical interpretation of the truncated expectations of ω_t^q is as follows: The function ϕ_t is the quantum-mechanical one-particle wave function of the Bose–Einstein condensate, while γ_t and σ_t describe the dynamics of sound waves in the quasifree approximation; in particular, $d(\gamma_t)$ determines the density of the “thermal cloud” of atoms. (In the physics literature, $n = d(\gamma)$ and $m = d(\sigma)$ are called the *non-condensate density* and *anomalous density*, respectively.)

The HFB Eqs. (24), (25) and (26) provide a *time-dependent extension* of the standard *stationary* Hartree–Fock–Bogoliubov equations for a Bose gas found in the physics literature; see, e.g., [9, 19, 21, 42]. Related equations (with $\phi_t = 0$) appear in superconductivity. These so-called *Bogoliubov-de Gennes* equations are equivalent to the BCS effective Hamiltonian description.

1.5. Summary of main results

The formulation of the nonlinear quasifree approximation in the form of Eq. (14), and the derivation of its equivalent formulations as self-consistent Eq. (16) for ω_t^q and the HFB Eqs. (39)–(43) for the truncated expectations ϕ, γ, σ , are among the main results presented in this paper; (see Theorems 2.2 and 2.3).

We also initiate a mathematical study of solutions of the HFB equations. In particular, if the initial state ω_0 is s.t. the operator γ_0 is trace-class (i.e., the number of atoms is finite) and σ_0 is Hilbert–Schmidt—for precise hypotheses see Sect. 2—we have the following results:

- Conservation of the total number of atoms in the gas:

$$\mathcal{N}(\phi_t, \gamma_t, \sigma_t) := \omega_t^q(\mathbb{N}), \quad (28)$$

where $\mathbb{N}$ is the particle-number operator; (see Corollary 2.5).

- Existence and conservation of the total energy (under suitable conditions on the two-body potential v and on the initial state ω_0^q):

$$\mathcal{E}(\phi_t, \gamma_t, \sigma_t) := \omega_t^q(\mathbb{H}) = \omega_0^q(\mathbb{H}), \quad (29)$$

i.e., $\mathcal{E}(\phi_t, \gamma_t, \sigma_t)$ is *independent* of t ; see Corollary 2.5 and Theorem 2.6, or Prop 3.12.

- *Positivity preservation property*: If $\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \geq 0$ at $t = 0$, then this holds for all times.
- Global well-posedness (Theorem 4.1) of the HFB equations.

It is in the proof of the local existence part of the last statement (Lemma 4.5(i)) that an error was made in [3]. In Lemma 4.5 (i) in Sect. 4 we prove the corresponding estimate under a more restrictive condition on the pair potential v - Condition (b') above.

In [7], the program outlined in [3] and this paper has been pursued for equations analogous to the HFB equations valid for fermions, namely the Bogoliubov-de Gennes equations; see also [17]. For references to related work see [7, 17].

We will show that any observable conserved by the von Neumann–Landau dynamics which is linear or quadratic in the creation- and annihilation operators is also conserved by the quasifree dynamics; see Theorem 2.4. In the special case of the observable $\mathbb{N}$, this yields the statement above. Energy conservation follows from Eq. (14), with $\mathbb{A} = \mathbb{H}_{\text{hfb}}(\omega_L^q)$, the quadratic nature of $\mathbb{H}_{\text{hfb}}(\omega_L^q)$, and Eq. (16).

Note that conservation of the total number of atoms in the gas is a consequence of (global) $U(1)$ -gauge invariance, i.e., invariance of the Hamiltonian $\mathbb{H}$ under the transformations

$$\psi(x) \rightarrow e^{i\theta} \psi(x), \quad \psi^*(x) \rightarrow e^{-i\theta} \psi^*(x), \quad \forall \theta \in \mathbb{R}, \forall x \in \mathbb{R}^d.$$

The total particle number, $\mathcal{N}(\phi, \gamma, \sigma) := \omega^q(\mathbb{N})$, and energy, $\mathcal{E}(\phi, \gamma, \sigma) := \omega^q(\mathbb{H})$, as functions of (ϕ, γ, σ) , can be evaluated explicitly:

$$\mathcal{N}(\phi, \gamma, \sigma) = \int (\gamma(x; x) + |\phi(x)|^2) dx. \quad (30)$$

The energy $\mathcal{E}(\phi, \gamma, \sigma)$ is given explicitly in Eq. (47). For a delta-function pair potential, $v = g\delta$, it takes the form

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \text{Tr}[h(\gamma + |\phi\rangle\langle\phi|)] \\ &\quad + g \int (2n(x)|\phi(x)|^2 + n(x)^2 + \frac{1}{2}|w(x)|^2) dx. \end{aligned} \quad (31)$$

(In terms of $\mathbb{H}_{\text{hfb}}(\omega^q)$, we have that $\mathcal{E}(\phi, \gamma, \sigma) := \omega^q(\mathbb{H}) = \omega^q(\mathbb{H}_{\text{hfb}}(\omega^q)) + \text{scalar}$.)

As usual, if γ is trace-class and σ is Hilbert–Schmidt the energy functional $\mathcal{E}$ can be used to give a variational characterization of stationary Gibbs states:

- Gibbs states minimize the energy $\mathcal{E}(\phi, \gamma, \sigma)$ under the constraint of constant entropy and for a fixed value of the expected particle number.

Equation (16) suggests to define *HFB stationary states* as the quasifree states satisfying the equation

$$\omega^q([\mathbb{A}, \mathbb{H}_{\text{hfb}}(\omega^q)]) = 0, \quad (32)$$

for all observables $\mathbb{A}$. (If ω^q is given by a density matrix, we can rewrite this equation as an explicit fixed point equation, see (33) below.) The most interesting ones among such states are the *ground states* and *Gibbs states*. These states are defined as:

$$\omega_{\beta, \mu}^q := \lim_{L \rightarrow \infty} \omega_L^q,$$

where ω_L^q is the quasifree ground state or Gibbs state of a Bose gas confined to a torus, $\Lambda_L = \mathbb{R}^d / 2L\mathbb{Z}^d$, i.e., to the box $[-L, L]^d$ with periodic boundary conditions. It satisfies the fixed point equation

$$\Phi_{\beta, \mu}(\omega_L^q) = \omega_L^q, \quad \text{with} \quad \Phi_{\beta, \mu}(\omega_L^q)(\mathbb{A}) := \text{Tr}[\mathbb{A} \exp(-\beta(\mathbb{H}_{\text{hfb}}(\omega_L^q) - \mu\mathbb{N}))] / \Xi, \quad (33)$$

where $\beta > 0$ is the inverse temperature, μ is the chemical potential, and the exponential of the negative pressure $\Xi = \text{Tr}[\exp(-\beta(\mathbb{H}_{\text{hfb}}(\omega_L^q)) - \mu\mathbb{N})]$ is the partition function of the gas. The quasifree state ω_L^q fulfilling (33) is a solution to Eq. (32) (or a stationary solution of Eq. (16)) for a gas confined to the box Λ_L . With regard to the thermodynamic limit, $L \rightarrow \infty$, we note that if the external potential V vanishes (i.e., for a translation-invariant Hamiltonian),

$$\omega^q([\mathbb{H}_{\text{hfb}}(\omega^q), \mathbb{A}]) := \lim_{L \rightarrow \infty} \omega_L^q([\mathbb{H}_{\text{hfb}}(\omega_L^q), \mathbb{A}]) = 0,$$

for any observable $\mathbb{A}$ localized in a compact region of position space.

Furthermore, if the external potential V vanishes (the translation-invariant case), one should replace the total energy and the particle number by the energy density and particle density, respectively, in order to study the approach to the thermodynamic limit, $L \rightarrow \infty$.

If $V = 0$ and γ and σ are translation-invariant, then the integrand in the energy functional $\mathcal{E}(\phi, \gamma, \sigma)$ (see (47)) is the energy density functional introduced in [18] and further studied in [38, 39]. It is shown in the latter papers that this functional has minimizers under the constraint of constant entropy- and particle densities. In [38, 39] it is also shown that a condensate appears in the corresponding minimizers. (To complete the picture one should show that the states thus obtained are stationary solutions to Eq. (16).)

In this paper, we do not consider the general problem of existence of static solutions. However, for $V = 0$, we present a result concerning existence of the positive-temperature, $U(1)$ -gauge- and translation-invariant HFB Gibbs states, and we show that Bose–Einstein condensation (BEC) occurs above a critical density; see Theorem 5.3.

As mentioned above, for $U(1)$ -gauge-invariant quasifree states, $\phi = 0$ and $\sigma = 0$; and hence HFB Gibbs states with these properties are, in fact, stationary solutions of the bosonic Hartree–Fock equation. Moreover, as the results of [38, 39] show, in the BEC regime, these states are not minimizers of the full HFB energy density, at fixed values of the entropy- and particle density. However, the existence of such states exhibiting Bose–Einstein condensation suggests that there are also $U(1)$ -symmetry breaking HFB Gibbs states with $\phi \neq 0$ and $\sigma \neq 0$.

1.6. Fixed point equation

Let $\mathbb{U}_{\omega^q}(t, s)$ denote the unitary propagator on bosonic Fock space $\mathcal{F}$, see (1), solving

$$i\partial_t \mathbb{U}_{\omega^q}(t, s) = \mathbb{H}_{\text{hfb}}(\omega_t^q) \mathbb{U}_{\omega^q}(t, s), \quad \text{with } \mathbb{U}_{\omega^q}(s, s) = \mathbf{1}, \forall s. \quad (34)$$

In terms of this propagator, we can rewrite Eq. (16), with initial condition $\omega_0^q = \omega_0$, as a fixed point problem,

$$\omega_t^q = \Phi_t(\omega_{(\cdot)}^q), \quad \text{with } \Phi_t(\omega_{(\cdot)}^q)(\mathbb{A}) := \omega_0^q(\mathbb{U}_{\omega^q}(t, 0)^* \mathbb{A} \mathbb{U}_{\omega^q}(t, 0)), \quad (35)$$

for all times $t \in \mathbb{R}$. Since the propagators $\mathbb{U}_{\omega^q}(t, s)$ are generated by families of quadratic Hamiltonians, we have that $\omega_0^q(\mathbb{U}_{\omega^q}(t, 0)^* \mathbb{A} \mathbb{U}_{\omega^q}(t, 0))$ is a quasifree state, for any time t . This formulation opens the possibility to prove existence of the quasifree dynamics directly, using a Brouwer–Schauder-type fixed-point theorem, without passing to the truncated expectations ϕ , γ and σ .

In this paper, we do not study whether the quasifree effective dynamics (16) (the HFB equations) provide an accurate approximation to the many-body dynamics (9), for finite times. There is a large literature concerning the derivation of the simpler Hartree- and Hartree–Fock equations from many-body dynamics in a limiting (mean-field) regime. Recently, evolution equations that include linear fluctuations around solutions of the Hartree equation (i.e., equations arising from linearization of the HFB equation in γ and σ) have been derived in [22, 23, 31–33, 36]; see [30] for a recent review, and [27] for an early contribution. Independently and in a different framework, equations equivalent to (39)–(41) are derived for *pure states* along with the conservation of particle number and energy in [22] and re-derived in a different way in [24]. For pure quasifree states, the relation $\gamma + \gamma^2 = \sigma \sigma^*$ holds, and Eqs. (39)–(41) turn out to be Hamiltonian evolution equations.

1.7. Organization of the paper

In Sect. 2, we first present the HFB equations, which we derive in Appendix 6. We then show that certain conservation laws for the many-body problem imply corresponding conservation laws for the HFB equation.

In Sect. 3, we show that the space of solutions of the HFB equations has a symplectic structure, and that these equations have similarities with Hamiltonian equations of motion.

In Sect. 3, we explain how the symplectic version of the HFB equations is related to the HFB eigenvalue equations found in the physics literature.

In Sect. 4, we prove that the Cauchy problem for the HFB equations is globally well-posed in the “energy space”, provided that the pair interaction potential is assumed to have suitable regularity properties. Our proof of global well-posedness is inspired in part by previous work on the Hartree–Fock equation [11, 12, 15, 16, 49]. We note that global existence for the related time-dependent Bogolubov-de Gennes equations for fermion systems has recently been established in [7], using a similar proof strategy.

In Sect. 5, we prove Bose–Einstein condensation for stationary states.

A brief summary of the theory of quasifree states and proofs of various technical lemmata is collected in Appendices.

2. The HFB equations and their basic properties

In this section, we formulate the HFB equations for a general pair potential v and prove the associated conservation laws. The derivation of the HFB equations is done in Appendix 6 by applying the quasifree reduction as in the introduction.

Definition of spaces. Let $M := \langle \nabla_x \rangle = \sqrt{1 - \Delta_x}$, with Δ_x being the Laplacian in d dimensions. We denote by $\mathcal{L}^1$ and $\mathcal{L}^2$ the spaces of trace-class and Hilbert–Schmidt operators on $L^2(\mathbb{R}^d)$ endowed with the trace norms $\|\cdot\|_{\mathcal{L}^1}$ and $\|\cdot\|_{\mathcal{L}^2}$, resp. For $j \in \mathbb{N}_0$ we define the spaces

$$X^j = H^j \oplus \mathcal{H}_\gamma^j \oplus \mathcal{H}_\sigma^j = \{(\phi, \gamma, \sigma) \in H^j \times \mathcal{H}_\gamma^j \times \mathcal{H}_\sigma^j\}, \quad (36)$$

with H^j being the Sobolev space $H^j(\mathbb{R}^d)$, $\mathcal{H}_\gamma^j := M^{-j} \mathcal{L}^1 M^{-j}$ being the space of trace-class operators γ such that $M^j \gamma M^j$ is also trace-class, and $\mathcal{H}_\sigma^j := \{\sigma \in \mathcal{L}^2 : \|M^j \sigma\|_{\mathcal{L}^2} + \|\sigma M^j\|_{\mathcal{L}^2} < \infty\}$ which may be viewed as the space of square-integrable functions σ on $\mathbb{R}^3 \times \mathbb{R}^3$ such that both $\langle \nabla_x \rangle^j \sigma$ and $\langle \nabla_y \rangle^j \sigma$ are square-integrable, too.

Defining the norms

$$\|\phi\|_{H^j} := \|M^j \phi\|_{L^2}, \quad \|\gamma\|_{\mathcal{H}_\gamma^j} := \|M^j \gamma M^j\|_{\mathcal{L}^1}, \quad \|\sigma\|_{\mathcal{H}_\sigma^j} := \|M^j \sigma\|_{\mathcal{L}^2} + \|\sigma M^j\|_{\mathcal{L}^2}, \quad (37)$$

on H^j , $\mathcal{H}_\gamma^j$, and $\mathcal{H}_\sigma^j$, respectively, we endow the spaces X^j with the norms

$$\|(\phi, \gamma, \sigma)\|_{X^j} = \|\phi\|_{H^j} + \|\gamma\|_{\mathcal{H}_\gamma^j} + \|\sigma\|_{\mathcal{H}_\sigma^j}$$

Furthermore, we let $\mathcal{X}_T := C^0([0, T]; X^3) \cap C^1([0, T]; X^1)$ and we denote by X_{qf}^j and $\mathcal{X}_T^{\text{qf}}$ the spaces of quasifree states and families of quasifree states with the 1st and 2nd order truncated expectations from the spaces X^j and $\mathcal{X}_T$, respectively.

Remark 2.1. For systems with infinite number of particles and finite density, one could replace $\mathbb{R}^d$ by the torus $\mathbb{T}_L^d := \mathbb{R}^d / (L\mathbb{Z})^d$ and then pass to the thermodynamic limit.

In what follows, we assume Conditions (a) and (b) stated in the Introduction [see Eqs. (5) and (6)].

Theorem 2.2. *The family of quasifree states $\omega_t^q \in \mathcal{X}_T^{\text{qf}}$ satisfies*

$$i \partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]) , \quad \forall \mathbb{A} \in \mathcal{A}^{(2)}, \quad (38)$$

with the Hamiltonian $\mathbb{H}$ defined in (4), if and only if the triple $(\phi_t, \gamma_t, \sigma_t) \in \mathcal{X}_T$ of the 1st and 2nd order truncated expectations of ω_t^q satisfies the time-dependent Hartree–Fock–Bogoliubov equations

$$i \partial_t \phi_t = h(\gamma_t) \phi_t + k(\sigma_t^{\phi_t}) \bar{\phi}_t, \quad (39)$$

$$i \partial_t \gamma_t = [h(\gamma_t^{\phi_t}), \gamma_t] + k(\sigma_t^{\phi_t}) \sigma_t^* - \sigma_t k(\sigma_t^{\phi_t})^*, \quad (40)$$

$$i \partial_t \sigma_t = [h(\gamma_t^{\phi_t}), \sigma_t]_+ + [k(\sigma_t^{\phi_t}), \gamma_t]_+ + k(\sigma_t^{\phi_t}), \quad (41)$$

where $[A_1, A_2]_+ = A_1 A_2^T + A_2 A_1^T$, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\sigma^\phi := \sigma + |\phi\rangle\langle\bar{\phi}|$, and

$$h(\gamma) = h + b[\gamma], \quad b[\gamma] := v * d(\gamma) + k(\gamma), \quad (42)$$

where

$$d(\gamma)(x) := \gamma(x, x), \quad k(\sigma) := v \sharp \sigma, \quad \text{and} \quad v \sharp \sigma(x, y) := v(x - y) \sigma(x, y). \quad (43)$$

If $v = g\delta$, then $h(\gamma)$ agrees with $h_{g\delta}(\gamma)$, and $k(\sigma)$ agrees with the multiplication operator by $g d(\sigma)(x)$, respectively, in (24)–(26).

Due to the fact that $h(\gamma_t)$ is Δ -bounded, for each $t > 0$, the r.h.s. of (39)–(41) belongs to the space X^0 . The proof of Theorem 2.2 is given in Appendix 6.

We now show that Eqs. (14) (or (39) to (41)) and (16) describing the quasifree dynamics are equivalent.

For a quasifree state ω^q with 1^{st} and 2^{nd} order truncated expectations $(\phi, \gamma, \sigma) \in X^1$, we define the quadratic Hamiltonian parametrized by (ϕ, γ, σ) as:

$$\begin{aligned} \mathbb{H}_{hfb}(\omega^q) &= \int \psi^*(x) h_v(\gamma) \psi(x) dx \\ &\quad - \int \psi^*(x) b[|\phi\rangle\langle\phi|] \phi(x) dx + h.c. \\ &\quad + \frac{1}{2} \int \psi^*(x) k[\sigma](x, y) \psi^*(y) dx dy + h.c. \end{aligned} \quad (44)$$

Theorem 2.3. Equation (14) is equivalent to the nonlinear, self-consistent evolution equation

$$i \partial_t \omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}_{hfb}(\omega_t^q)]), \quad (45)$$

defined for all observables $\mathbb{A}$. The equivalence holds for observables linear or quadratic in creation- and annihilation operators.

Moreover, truncated expectations $(\phi_t, \gamma_t, \sigma_t) \in \mathcal{X}_T$ satisfy the HFB Eqs. (39) to (41) if and only if the corresponding quasifree state $\omega_t^q \in \mathcal{X}_T^{\text{qf}}$ satisfies (45).

The proof of Theorem 2.3 is given in Appendix C.

We now prove the conservation laws for the number of particles (or more generally, for any observable commuting with the Hamiltonian $\mathbb{H}$ which is quadratic with respect to creation and annihilation operators), and for the energy.

Theorem 2.4. Assume that an observable $\mathbb{A} \in \mathcal{A}^{(2)}$ satisfies $[\mathbb{H}, \mathbb{A}] = 0$. Then, $\omega_t^q(\mathbb{A})$ is conserved:

$$\omega_t^q(\mathbb{A}) = \omega_0^q(\mathbb{A}) \quad \forall t \in \mathbb{R}. \quad (46)$$

Proof. This follows from (38) for $\mathbb{A}$ of order up to two, with $[\mathbb{A}, \mathbb{H}] = 0$. $\square$

To draw some consequences from this result, we need to define additional spaces.

Corollary 2.5. Let $\omega_t^q \in \mathcal{X}_T^{\text{qf}}$ solve (38) (or (45)). Then, the number of particles $\mathcal{N}(\phi_t, \gamma_t, \sigma_t) = \omega_t^q(\mathbb{N})$ and the energy $\omega_t^q(\mathbb{H})$ are conserved.

Theorem 2.6. *Let $\omega^q \in X^{\text{qf}}$. Then, the energy $\omega^q(\mathbb{H}) = \mathcal{E}(\phi, \gamma, \sigma)$ is given explicitly as:*

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \text{Tr}[h(\gamma + |\phi\rangle\langle\phi|)] + \text{Tr}[b[|\phi\rangle\langle\phi|]\gamma] \\ &+ \frac{1}{2}\text{Tr}[b[\gamma]\gamma] + \frac{1}{2} \int v(x-y)|\sigma(x, y) + \phi(x)\phi(y)|^2 dx dy. \end{aligned} \quad (47)$$

Proof. We use

$$\omega_C^q(\mathbb{A}) := \omega^q(W_\phi \mathbb{A} W_\phi^*), \quad (48)$$

where the Weyl operators are defined through $W_\phi = \exp(\psi^*(\phi) - \psi(\phi))$ and satisfy

$$W_\phi^* \psi(x) W_\phi = \psi(x) + \phi(x). \quad (49)$$

Note that the state $\omega_{C,t}^q$ is quasifree because ω^q is quasifree. By construction $\omega_C^q(\psi(x)) = 0$ and thus using (10) and the quasifreeness of ω_C^q , one sees that ω_C^q vanishes on monomials of odd order in the creation and annihilation operators. Note that $\mathcal{E}(\phi, \gamma, \sigma) = \omega_C^q(W_\phi^* \mathbb{H} W_\phi)$, hence using the vanishing on monomials of odd order in the creation and annihilation operators

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \omega_{C,t}^q \left(\int v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y) dx dy \right. \\ &\quad + \frac{1}{2} \left(\int v(x-y) \phi_t(x) \phi_t(y) \psi^*(x) \psi^*(y) dx dy + h.c. \right) \\ &\quad + \int (h + b[|\phi\rangle\langle\phi|])(x; y) \psi^*(x) \psi(y) dx dy \Big) \\ &\quad + \frac{1}{2} \int |\phi(x)\phi(y)|^2 v(x-y) dx dy + \langle \phi, h\phi \rangle. \end{aligned}$$

Then, using that ω_C^q is a quasifree state with expectations $(0, \gamma, \sigma)$ yields

$$\begin{aligned} \mathcal{E}(\phi, \gamma, \sigma) &= \frac{1}{2} \text{Tr}[b[\gamma]\gamma] + \frac{1}{2} \int \overline{\sigma(x, y)} v(x-y) \sigma(x, y) dx dy \\ &\quad + \Re \left(\int \overline{\sigma(x, y)} v(x-y) \phi(x) \phi(y) dx dy \right) \\ &\quad + \text{Tr}[(h + b[|\phi\rangle\langle\phi|])\gamma] + \frac{1}{2} \int |\phi(x)\phi(y)|^2 v(x-y) dx dy + \langle \phi, h\phi \rangle \end{aligned}$$

which gives the expression of the energy in terms of ϕ, γ and σ .

3. Generalized one-particle density matrix and Bogoliubov transforms

In this section, we consider the HFB Eqs. (40)–(41) for γ_t and σ_t and reformulate them in terms the generalized one-particle density matrix $\Gamma_t = \begin{pmatrix} \gamma_t & \sigma_t \\ \bar{\sigma}_t & 1 + \bar{\gamma}_t \end{pmatrix}$. We show

that the diagonalizing maps for Γ_t are symplectomorphisms (see below for the definition) and that the resulting equation for Γ_t is equivalent to the evolution equation for these symplectomorphisms. The latter will allow us to (a) give another proof of the conservation of energy without using the second quantization framework and (b) connect the time-dependent HFB Eqs. (40)–(41) to the time-independent HFB equations used in the physics literature. See Sect. 3.

We begin by relating properties of $\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix}$ to those of γ and σ .

Proposition 3.1. *The generalized one-particle density matrix, Γ , is nonnegative,*

$$\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \geq 0, \quad (50)$$

iff the following four conditions 1. – 4. are fulfilled,

1. The operator $\gamma \geq 0$ is positive semidefinite.
2. The expectation $\sigma(x, y) = \sigma(y, x)$ is symmetric.
3. The inequality $\sigma(1 + \bar{\gamma})^{-1}\sigma^* \leq \gamma$ holds true in the sense of quadratic forms.
4. The bound $\frac{1}{2}\|\sigma\|_{\mathcal{H}_\sigma^1}^2 \leq \|\gamma\|_{\mathcal{H}_\gamma^1}(1 + \text{Tr}[\gamma])$ holds true.

(Statement (4) follows from (1) and (3) and is given here for later convenience of references.)

Proof. We remark that the truncated expectations γ and σ are the expectations of the state

$$\omega_C(\mathbb{A}) := \omega(W_\phi \mathbb{A} W_\phi^*)$$

where $W_\phi = \exp(\psi^*(\phi) - \psi(\phi))$ are the Weyl operators. W_ϕ satisfy $W_\phi \psi(x) W_\phi^* = \psi(x) - \phi(x)$. The generalized one particle density matrix Γ of ω_C is non-negative, since, for all f, g in L^2 ,

$$\left\langle \begin{pmatrix} f \\ g \end{pmatrix}, \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \begin{pmatrix} f \\ g \end{pmatrix} \right\rangle = \omega_C((\psi^*(f) + \psi(\bar{g}))(\psi(f) + \psi^*(\bar{g}))) \geq 0. \quad (51)$$

Statements (1) and (2) are obvious. The inequality in Point (3) follows from the Schur complement argument:

$$\begin{aligned} 0 &\leq \begin{pmatrix} 1 - \sigma(1 + \bar{\gamma})^{-1} & \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \gamma & \sigma \\ \sigma^* & 1 + \bar{\gamma} \end{pmatrix} \begin{pmatrix} 1 - \sigma(1 + \bar{\gamma})^{-1} \\ 0 & 1 \end{pmatrix}^* \\ &= \begin{pmatrix} \gamma - \sigma(1 + \bar{\gamma})^{-1}\sigma^* & 0 \\ 0 & 1 + \bar{\gamma} \end{pmatrix}. \end{aligned}$$

Finally, we observe that (1) and (3) and the inequality $\gamma \leq \text{Tr}[\gamma]\mathbf{1}$ imply the following bound on $\sigma\sigma^*$,

$$(1 + \text{Tr}[\gamma])^{-1}\sigma\sigma^* \leq \sigma(1 + \bar{\gamma})^{-1}\sigma^* \leq \gamma.$$

Inserting $M = \sqrt{1 - \Delta_x}$ on both sides and taking the trace yields (4). $\square$

Notations. With the spaces and norms defined in (36)–(37) and for $j \in \mathbb{N}_0$ we define the spaces

$$Y^j = \mathcal{K}_\gamma^j \oplus \mathcal{K}_\sigma^j, \quad (52)$$

with the norms on Y^j given by

$$\|(\gamma, \sigma)\|_{Y^j} = \|\gamma\|_{\mathcal{K}_\gamma^j} + \|\sigma\|_{\mathcal{K}_\sigma^j}.$$

We also use the spaces $\mathcal{Y}_T := C^0([0, T]; Y^3) \cap C^1([0, T]; Y^1)$ and $\tilde{\mathcal{Y}}_T :=$ the space of generalized one-particle density matrices, Γ , with entries in $\mathcal{Y}_T$.

In what follows we fix a number $T > 0$ and a family $\phi_t \in C^0([0, T]; H^3) \cap C^1([0, T]; H^1)$ (not necessarily a solution of (39)) and do not display it in our notation. A simple computation yields the first result of this section:

Proposition 3.2. $(\gamma_t, \sigma_t) \in \mathcal{Y}_T$ is a solution to the HFB Eqs. (40)–(41) iff $\Gamma_t = \begin{pmatrix} \gamma_t & \sigma_t \\ \bar{\sigma}_t & 1 + \bar{\gamma}_t \end{pmatrix} \in \tilde{\mathcal{Y}}_T$ solves the equation

$$i \partial_t \Gamma_t = \mathcal{S} \Lambda(\Gamma_t) \Gamma_t - \Gamma_t \Lambda(\Gamma_t) \mathcal{S}, \quad (53)$$

with $\Lambda(\Gamma) = \begin{pmatrix} h(\gamma^\phi) & k(\sigma^\phi) \\ k(\sigma^\phi) & h(\gamma^\phi) \end{pmatrix}$, where, recall, $h(\gamma)$ and $k(\sigma)$ are defined in (42) and (43), and $\mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.

To formulate the next result, we introduce some definitions.

Definition 3.3. Let $\mathfrak{h}$ denote a complex Hilbert space. A bounded linear operator $\mathcal{U} = \begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix}$ on $\mathfrak{h} \oplus \mathfrak{h}$ with the property that

$$\mathcal{U}^* \mathcal{S} \mathcal{U} = \mathcal{S} \quad \text{and} \quad \mathcal{U} \mathcal{S} \mathcal{U}^* = \mathcal{S}, \quad (54)$$

where $\mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, is called a symplectomorphism.

If, moreover, there exists a unitary transformation $\mathbb{U}$ on Fock space, sometimes called implementation of $\mathcal{U}$, such that

$$\forall f, g \in \mathfrak{h}, \quad \mathbb{U}[\psi^*(f) + \psi(\bar{g})] \mathbb{U}^* = \psi^*(uf + vg) + \psi(v\bar{f} + u\bar{g}),$$

then the symplectomorphism $\mathcal{U}$ is said to be implementable.

Remark 3.4. The operator $\mathcal{U}$ is a symplectomorphism in the sense that it preserves the symplectic form $\text{Im} \langle \cdot, \mathcal{S} \cdot \rangle$ on $\mathfrak{h} \oplus \mathfrak{h}$ (i.e., is a canonical map). (In fact, $\mathcal{U}$ preserves $\langle \cdot, \mathcal{S} \cdot \rangle$.)

Remark 3.5. The operator $\mathcal{U}$ is a symplectomorphism if and only if the operator $f \mapsto uf + v\bar{f}$ is a symplectomorphism on $(\mathfrak{h}, \text{Im} \langle \cdot, \cdot \rangle)$ in the usual sense (i.e., it preserves the symplectic form $\text{Im} \langle \cdot, \cdot \rangle$).

Remark 3.6. The conditions in (54) are equivalent to satisfying the four equations

$$uu^* - vv^* = \mathbf{1}, \quad u^*u - v^T \bar{v} = \mathbf{1}, \quad u^*v = v^T \bar{u}, \quad uv^T = vu^T. \quad (55)$$

Remark 3.7. The transformation

$$\forall f, g \in \mathfrak{h}, \quad (\psi^*(f), \psi(\bar{f})) \rightarrow (\psi^*(uf) + \psi(v\bar{f}), \psi^*(vf) + \psi(u\bar{f})) \quad (56)$$

is called a Bogoliubov transformation. It is easy to check that it preserves the CCR iff the operator $\mathcal{U} = \begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix}$ satisfies (54).

If v is Hilbert–Schmidt, then the Bogoliubov transformation (56) is implementable. This condition is referred to as the Shale condition; see [47].

For later use, we introduce the Banach space

$$\mathcal{H}^{\infty,2} = \left\{ \begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix} \mid a \in \mathcal{B}(H^1) \simeq M\mathcal{B}(\mathfrak{h})M^{-1}, \quad b \in M\mathcal{L}^2M^{-1} \right\},$$

where $\mathcal{B}(E)$ denotes the (Banach) space of bounded operators on a Banach space E . $\mathcal{H}^{\infty,2}$ is endowed with the norm $\left\| \begin{pmatrix} a & b \\ \bar{b} & \bar{a} \end{pmatrix} \right\|_{\mathcal{H}^{\infty,2}} = \|a\|_{\mathcal{B}(H^1)} + \|b\|_{M\mathcal{L}^2M^{-1}}$, using the same identification between operators and kernels as before.

We begin with an auxiliary result:

Proposition 3.8. *Let $\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1+\bar{\gamma} \end{pmatrix} \in Y^1$ and $\Gamma \geq 0$. Then, there exist an implementable symplectomorphism $\mathcal{U} \in \mathcal{H}^{\infty,2}$ such that*

$$\Gamma = \mathcal{U} \begin{pmatrix} \gamma' & 0 \\ 0 & 1 + \bar{\gamma}' \end{pmatrix} \mathcal{U}^*,$$

where $0 \leq \gamma' \leq \gamma$. The operator γ' is unique up to conjugation by a unitary operator.

This result is related to Theorem 1 of [37], which is stronger. See also [5, 8]. As the relation between the two results is not obvious, we give a direct proof of Proposition 3.8 after the proof of Proposition 3.9.

The next result relates the evolution of Γ_t to the evolution of implementable symplectomorphisms $\mathcal{U}_t \in \mathcal{H}^{\infty,2}$ that diagonalize Γ_t .

Proposition 3.9. (i) *For any $\Gamma_t \in \tilde{\mathcal{Y}}_T$ and any implementable symplectomorphism $\mathcal{U}_0 \in \mathcal{H}^{\infty,2}$, the initial value problem*

$$i\partial_t \mathcal{U}_t^* = \mathcal{S}\Lambda(\Gamma_t)\mathcal{U}_t^*, \quad \mathcal{U}_{t=0} = \mathcal{U}_0, \quad (57)$$

has a unique solution in $\mathcal{H}^{\infty,2}$, which is a symplectomorphism for every t .

(ii) *Let $\Gamma_t \in \tilde{\mathcal{Y}}_T$ solve Eq. (53), with an initial condition $\Gamma_0 \in \tilde{Y}^3$, s.t. $\Gamma_0 \geq 0$. Let $\mathcal{U}_0$ be an implementable symplectomorphism diagonalizing Γ_0 ,*

$$\Gamma_0 = \mathcal{U}_0 \Gamma'_0 \mathcal{U}_0^*, \quad \Gamma'_0 = \begin{pmatrix} \gamma'_0 & 0 \\ 0 & 1 + \bar{\gamma}'_0 \end{pmatrix}.$$

Then, the continuous family of implementable symplectomorphisms $\mathcal{U}_t$ in $\mathcal{H}^{\infty,2}(\mathfrak{h} \times \mathfrak{h})$ satisfying (57), with the above $\mathcal{U}_0$, diagonalizes Γ_t :

$$\Gamma_t = \mathcal{U}_t^* \Gamma'_0 \mathcal{U}_t \geq 0. \quad (58)$$

Proof of Prop. 3.9. The operator $\Lambda(\Gamma_t)$ can be decomposed as $\Lambda(\Gamma_t) = \Lambda_1 + \Lambda_{2,t}$ with

$$\Lambda_1 = \begin{pmatrix} h & 0 \\ 0 & \bar{h} \end{pmatrix}, \quad \Lambda_{2,t} = \begin{pmatrix} b[\gamma_t + |\phi_t\rangle\langle\phi_t|] & k[\sigma_t + \phi_t \otimes \phi_t] \\ k[\sigma_t + \phi_t \otimes \phi_t] & b[\gamma_t + |\phi_t\rangle\langle\phi_t|] \end{pmatrix}.$$

The first operator, Λ_1 , is the generator of a continuous one-parameter group in $\mathcal{H}^{\infty,2}$. As for the second one, using the continuity of $t \mapsto \Gamma_t \in Y^1$ and Lemma 4.5, we get the continuity of $t \mapsto \Lambda_{2,t} \in \mathcal{H}^{\infty,2}$. We can thus use classical results of functional analysis (see, e.g., [28]) to obtain the existence and uniqueness of $\mathcal{U}_t$ and its regularity.

The same arguments as in the next lemma prove that $\mathcal{U}_t$ is a symplectomorphism.

Finally, Γ_t and $\mathcal{U}_t^* \Gamma_0 \mathcal{U}_t$ satisfy the same differential equation, and the uniqueness of a solution to (57) proves the last equality. $\square$

Proof of existence in Prop. 3.8 We split the proof into two lemmata, Lemmata 3.10, establishing local existence, and 3.11, proving global existence, below. The strategy is to construct Γ_t and symplectomorphisms $\mathcal{U}_t$ such that $\mathcal{U}_t \Gamma_t \mathcal{U}_t^* = \Gamma_0$, for all t , and in the limit $t \rightarrow \infty$, Γ_∞ has the desired form. The key step will be to use a differential equation for Γ_t implying $\|\sigma_t\|_{\mathcal{H}_\sigma^1} \searrow 0$. $\square$

Lemma 3.10. (i) Let $T > 0$ and $t \mapsto \Lambda_t = \begin{pmatrix} a_t & b_t \\ \bar{b}_t & \bar{a}_t \end{pmatrix} \in C([0, T]; \mathcal{H}^{\infty,2})$. Then, the ordinary differential equation

$$i \partial_t \mathcal{U}_t^* = \mathcal{S} \Lambda_t \mathcal{U}_t^*, \quad (59)$$

with initial data $\mathcal{U}_0^* = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, has a unique global solution $\mathcal{U}_t \in C^1([0, T]; \mathcal{H}^{\infty,2})$, and $\mathcal{U}_t$ is a symplectomorphism for all time.

(ii) Moreover, if $\gamma_t \in C^1([0, T]; \mathcal{H}_\gamma^1)$, $\sigma_t \in C^1([0, T]; \mathcal{H}_\sigma^1)$ satisfy

$$i \partial_t \gamma_t = a_t \gamma_t - b_t \bar{\sigma}_t - \gamma_t a_t + \sigma_t \bar{b}_t, \quad (60)$$

$$i \partial_t \sigma_t = a_t \sigma_t - b_t (1 + \bar{\gamma}_t) - \gamma_t b_t + \sigma_t \bar{a}_t, \quad (61)$$

with initial data $\sigma_0 = \sigma$, $\gamma_0 = \gamma$ given in Prop 3.9(i), then, for all time $t \in [0, T]$,

$$\mathcal{U}_t \Gamma_t \mathcal{U}_t^* = \Gamma_0. \quad (62)$$

Proof. The existence and uniqueness of $\mathcal{U}_t^*$ follows from the theory of time-dependent linear ordinary differential equations once one observes that $\mathcal{H}_\gamma^1$ and $\mathcal{H}_\sigma^1$ are continuously embedded in $\mathcal{B}(H^1)$ and $M\mathcal{L}^2(L^2)M^{-1}$. At $t = 0$, $\mathcal{U}_0 \mathcal{S} \mathcal{U}_0^* = \mathcal{S}$ and

$$i \partial_t (\mathcal{U}_t \mathcal{S} \mathcal{U}_t^*) = \mathcal{U}_t (-\Lambda_t \mathcal{S} \mathcal{S} + \mathcal{S} \mathcal{S} \Lambda_t) \mathcal{U}_t^* = 0,$$

thus $\mathcal{U}_t \mathcal{S} \mathcal{U}_t^* = \mathcal{S}$ for all time, and, to prove $\mathcal{U}_t^* \mathcal{S} \mathcal{U}_t = \mathcal{S}$, one observes that

$$i \partial_t (\mathcal{U}_t^* \mathcal{S} \mathcal{U}_t) = -(\mathcal{U}_t^* \mathcal{S} \mathcal{U}_t) \Lambda_t \mathcal{S} + \mathcal{S} \Lambda_t (\mathcal{U}_t^* \mathcal{S} \mathcal{U}_t),$$

which is a linear time-dependent ordinary differential equation for $\mathcal{U}_t^* \mathcal{S} \mathcal{U}_t$ which also admits the constant solution $\mathcal{S}$. By uniqueness of the solution, one gets that $\mathcal{U}_t^* \mathcal{S} \mathcal{U}_t = \mathcal{S}$. Hence, $\mathcal{U}_t$ is a symplectomorphism for all time.

Similarly, the derivative $i \partial_t (\mathcal{U}_t \Gamma_t \mathcal{U}_t^*)$ vanishes because, using (60) and (61),

$$i \partial_t \Gamma_t = \Lambda_t \mathcal{S} \Gamma_t - \Gamma_t \mathcal{S} \Lambda_t.$$

Thus $\mathcal{U}_t \Gamma_t \mathcal{U}_t^* = \mathcal{U}_0 \Gamma_0 \mathcal{U}_0^* = \Gamma_0$ for all times. $\square$

We choose a_t and b_t in (60) and (61) such that σ_t vanishes in the limit $t \rightarrow \infty$. Let $\mathcal{L}^1(\mathfrak{h})$ and $\mathcal{L}^2(\mathfrak{h})$ denote the spaces of trace-class and Hilbert–Schmidt operators, resp., on the space $\mathfrak{h}$.

Lemma 3.11. (i) *The ordinary differential equation*

$$\partial_t \gamma_t = -2\sigma_t \bar{\sigma}_t, \quad (63)$$

$$\partial_t \sigma_t = -(\sigma_t + \sigma_t \bar{\gamma}_t + \gamma_t \sigma_t), \quad (64)$$

with initial data $\sigma_0 = \sigma$, $\gamma_0 = \gamma$ given in Prop. 3.9(i), has a unique global solution $(\gamma_t, \sigma_t) \in C^1([0, \infty); \mathcal{L}^1(\mathfrak{h}) \times \mathcal{L}^2(\mathfrak{h}))$.

(ii) *Given the solution $(\gamma_t, \sigma_t) \in C^1([0, \infty); \mathcal{L}^1(\mathfrak{h}) \times \mathcal{L}^2(\mathfrak{h}))$ from (i), let $\Lambda_t = \begin{pmatrix} 0 & i\sigma_t \\ -i\bar{\sigma}_t & 0 \end{pmatrix}$, $\mathcal{U}_t = \begin{pmatrix} u_t & v_t \\ \bar{v}_t & \bar{u}_t \end{pmatrix}$ and $\Gamma_t = \begin{pmatrix} \gamma_t & \sigma_t \\ \bar{\sigma}_t & 1 + \bar{\gamma}_t \end{pmatrix}$ be as in Lemma 3.10. Then, $\mathcal{U}_t$ converges in $\mathcal{H}^{\infty,2}$ to a symplectomorphism $\mathcal{U}_\infty$ and*

$$\Gamma_0 = \mathcal{U}_\infty \Gamma_\infty \mathcal{U}_\infty^* = \mathcal{U}_\infty \begin{pmatrix} \gamma_\infty & 0 \\ 0 & 1 + \bar{\gamma}_\infty \end{pmatrix} \mathcal{U}_\infty^*,$$

with $0 \leq \gamma_\infty \leq \gamma_0$.

Proof. The existence of maximal solutions to (63)–(64) follows from the Picard–Lindelöf theorem. Now using the $\mathcal{U}_t$ constructed in Lemma (3.10), one gets that $(\mathcal{U}_t)^{-1} \Gamma_0 (\mathcal{U}_t^*)^{-1} = \Gamma_t$, which implies that $\Gamma_t \geq 0$ and thus $\gamma_t \geq 0$. It then follows from (63) that γ_t is decreasing in the sense of quadratic forms and $\|\gamma_t\|_{\mathcal{H}_\gamma^1} \leq \|\gamma_0\|_{\mathcal{H}_\gamma^1}$.

One first obtains an estimate on $\|\sigma_t\|_{\mathcal{L}^2}^2 = \text{Tr}[\sigma_t \sigma_t^*]$, using (64):

$$\begin{aligned} \partial_t \|\sigma_t\|_{\mathcal{L}^2}^2 &= \text{Tr}[-(\sigma_t + \sigma_t \bar{\gamma}_t + \gamma_t \sigma_t) \sigma_t^* - \sigma_t (\sigma_t^* + \bar{\gamma}_t \sigma_t^* + \sigma_t^* \gamma_t)] \\ &\leq -2 \text{Tr}[\sigma_t \sigma_t^*] = -2 \|\sigma_t\|_{\mathcal{L}^2}^2. \end{aligned}$$

This implies that $\|\sigma_t\|_{\mathcal{L}^2} \leq \|\sigma_0\|_{\mathcal{L}^2} \exp(-t)$. Using again (64) and the fact that $\gamma_t \geq 0$ one finds that

$$\begin{aligned} \partial_t \|\sigma_t\|_{\mathcal{H}_\sigma^1}^2 &= \text{Tr}[-(\sigma_t + \sigma_t \bar{\gamma}_t + \gamma_t \sigma_t) \sigma_t^* M^2 - \sigma_t (\sigma_t^* + \bar{\gamma}_t \sigma_t^* + \sigma_t^* \gamma_t) M^2] \\ &\leq -2 \|\sigma_t\|_{\mathcal{H}_\sigma^1}^2 - \text{Tr}[\gamma_t \sigma_t \sigma_t^* M^2] - \text{Tr}[\sigma_t \sigma_t^* \gamma_t M^2] \end{aligned}$$

We remark that $|\text{Tr}[M \gamma_t \sigma_t \sigma_t^* M]| \leq \|\gamma_t\|_{\mathcal{H}_\gamma^1}^{1/2} \|\gamma_t\|_{\mathcal{B}(\mathfrak{h})}^{1/2} \|\sigma_t\|_{\mathcal{H}_\sigma^1}$ and

$$\|\gamma_t\|_{\mathcal{B}(\mathfrak{h})}^{1/2} \|\sigma_t\|_{\mathcal{B}(\mathfrak{h})} \leq \|\gamma_t\|_{\mathcal{L}^2}^{1/2} \|\sigma_t\|_{\mathcal{L}^2} \leq \|\gamma_0\|_{\text{Tr}}^{1/2} \|\sigma_0\|_{\mathcal{L}^2} e^{-t},$$

hence

$$\partial_t \|\sigma_t\|_{\mathcal{H}_\sigma^1}^2 \leq -2\|\sigma_t\|_{\mathcal{H}_\sigma^1}^2 + \sqrt{2C}e^{-t} \sqrt{2}\|\sigma_t\|_{\mathcal{H}_\sigma^1} \leq -\|\sigma_t\|_{\mathcal{H}_\sigma^1}^2 + Ce^{-2t}$$

which yields $\|\sigma_t\|_{\mathcal{H}_\sigma^1}^2 \leq Ce^{-t}\|\sigma_0\|_{\mathcal{H}_\sigma^1}^2$. The pair (γ_t, σ_t) is thus bounded in $\mathcal{H}_\gamma^1 \oplus \mathcal{H}_\sigma^1$ and the maximal time of the solution is $T = \infty$. We also get that $\gamma_t \rightarrow \gamma_\infty$ in $\mathcal{H}_\gamma^1$ as $t \rightarrow \infty$ as γ_t is decreasing and bounded below, and $\sigma_t \rightarrow 0$.

Integrating the derivative of $\mathcal{U}_t^*$ and taking the norm of both sides yields

$$\|\mathcal{U}_t^*\|_{\mathcal{H}^{\infty,2}} \leq \|\mathcal{U}_0^*\|_{\mathcal{H}^{\infty,2}} + \int_0^t \|\sigma_s\|_{\mathcal{H}_\sigma^1} \|\mathcal{U}_s^*\|_{\mathcal{H}^{\infty,2}} ds. \quad (65)$$

The Grönwall lemma, combined with $\|\mathcal{U}_0^*\|_{\mathcal{H}^{\infty,2}} = 1$ and the estimate on $\|\sigma_t\|_{\mathcal{H}_\sigma^1}$ provide

$$\|\mathcal{U}_t^*\|_{\mathcal{H}^{\infty,2}} \leq \exp\left(\int_0^t \|\sigma_s\|_{\mathcal{H}_\sigma^1} ds\right) \leq \exp(C\|\sigma_0\|_{\mathcal{H}_\sigma^1}).$$

Thus, the integral $\int_0^\infty \mathcal{S}\Lambda_s \mathcal{U}_s^* ds$ is absolutely convergent and

$$\mathcal{U}_t^* \xrightarrow[t \rightarrow \infty]{} \mathcal{U}_0^* - i \int_0^\infty \mathcal{S}\Lambda_s \mathcal{U}_s^* ds =: \mathcal{U}_\infty^*$$

in $\mathcal{H}^{\infty,2}$, and the limit $\mathcal{U}_\infty^*$ is still an implementable symplectomorphism.

Hence,

$$\Gamma_0 - \mathcal{U}_\infty \Gamma_\infty \mathcal{U}_\infty^* = \mathcal{U}_t \Gamma_t \mathcal{U}_t^* - \mathcal{U}_\infty \Gamma_\infty \mathcal{U}_\infty^* \rightarrow 0$$

as $t \rightarrow \infty$, where $\Gamma_\infty = \begin{pmatrix} \gamma_\infty & 0 \\ 0 & 1+\bar{\gamma}_\infty \end{pmatrix}$, and the convergence takes place in the space of block operators with diagonal elements in $\mathcal{H}_\gamma^1$ and off-diagonal elements in $\mathcal{H}_\sigma^1$. This proves the last point. $\square$

This completes the proof of existence. $\square$

Proof of uniqueness in Prop. 3.8 Indeed, let us consider γ' and γ'' satisfying the conditions of Prop. 3.8. Then, there exists a symplectomorphism $\mathcal{U}$ such that $\begin{pmatrix} \gamma'' & 0 \\ 0 & \bar{\gamma}''+1 \end{pmatrix} = \mathcal{U}^* \begin{pmatrix} \gamma' & 0 \\ 0 & \bar{\gamma}'+1 \end{pmatrix} \mathcal{U}$. As $\mathcal{U}^* \mathcal{S} \mathcal{U} = \mathcal{S}$, this is equivalent to

$$\begin{pmatrix} \gamma'' + 1/2 & 0 \\ 0 & \bar{\gamma}'' + 1/2 \end{pmatrix} = \mathcal{U}^* \begin{pmatrix} \gamma' + 1/2 & 0 \\ 0 & \bar{\gamma}' + 1/2 \end{pmatrix} \mathcal{U} \quad (66)$$

and we want to prove that γ' and γ'' are unitarily equivalent in L^2 . The off-diagonal entries in (66) yield $u^*(\gamma' + 1/2)v + v^T(\gamma' + 1/2)\bar{u} = 0$ and as $\mathcal{U}$ is a symplectomorphism, we get from (55) that u is invertible and $v\bar{u}^{-1} = u^{*-1}v^T$. Thus,

$$(\gamma' + \frac{1}{2})v\bar{u}^{-1} + v\bar{u}^{-1}(\gamma' + \frac{1}{2}) = 0.$$

We can now use a known method to solve the Lyapunov (or Sylvester) equations:

$$\begin{aligned} v\bar{u}^{-1} &= - \int_0^\infty \frac{d}{dt} \left(e^{-t(\gamma' + \frac{1}{2})} v\bar{u}^{-1} e^{-t(\gamma' + \frac{1}{2})} \right) dt \\ &= \int_0^\infty e^{-t(\gamma' + \frac{1}{2})} \left((\gamma' + \frac{1}{2}) v\bar{u}^{-1} + v\bar{u}^{-1} (\gamma' + \frac{1}{2}) \right) e^{-t(\gamma' + \frac{1}{2})} dt = 0, \end{aligned}$$

where we used that $\gamma + 1/2 \geq 1/2$, so that there is no problem in handling the integrals. Hence $v = 0$, and, using (55) again, u is a unitary operator. And thus $\gamma'' = u^* \gamma' u$ which proves the result. $\square$

We now write the HFB equations in a form that is reminiscent of a Hamiltonian structure, and use it to give a direct proof of the conservation of the energy.

Notation: For $\phi \in H^1$, $\mathcal{U} = \begin{pmatrix} u & v \\ \bar{v} & \bar{u} \end{pmatrix} \in \mathcal{H}^{\infty,2}$ a symplectomorphism, and $\gamma'_0 \in \mathcal{H}^1$ non-negative. We set

$$\begin{aligned} \mathcal{H}_{\gamma'_0}(\phi, u, v) &:= \langle \phi, h\phi \rangle + \text{Tr}[(u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v})(h + b[|\phi\rangle\langle\phi|])] \\ &\quad + \frac{1}{2} \text{Tr}[(u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v}) b[u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v}]] \\ &\quad + \frac{1}{2} \text{Tr}[k[u^* \gamma'_0 v + v^T (1 + \bar{\gamma}'_0) \bar{u} + |\phi\rangle\langle\bar{\phi}|](v^* \gamma'_0 u + u^T (1 + \bar{\gamma}'_0) \bar{v} + |\bar{\phi}\rangle\langle\phi|)]. \end{aligned}$$

In the next proposition and its proof we use the abbreviations $h(t) \equiv h(\gamma_t^{\phi_t})$ and $k(t) \equiv k(\sigma_t^{\phi_t})$, where, recall, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\sigma^\phi := \sigma + \phi \otimes \phi$, and $h(\gamma)$ and $k(\sigma)$ are defined in (42) and (43).

Proposition 3.12. *Let $\rho_t = (\phi_t, \gamma_t, \sigma_t) \in C^0([0, T]; X^3) \cap C^1([0, T]; X^1)$ be a solution to the HFB Eqs. (39)–(41) in the classical sense, on an interval $[0, T)$, with $T > 0$. Let $\mathcal{U}_t$ and γ'_0 be as in Proposition 3.9.*

Then, $\mathcal{E}(\phi_t, \gamma_t, \sigma_t) = \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t)$ and the derivatives of $\mathcal{H}_{\gamma'_0}$ and of (ϕ_t, u_t, v_t) are linked through the equations

$$\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \bar{\phi}}(\phi_t, u_t, v_t) = i \partial_t \phi_t, \quad (67)$$

$$\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi_t, u_t, v_t) = \gamma'_0 i \partial_t u_t + \frac{1}{2} v_t \overline{k(t)}, \quad (68)$$

$$\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi_t, u_t, v_t) = -\gamma'_0 i \partial_t v_t + v_t \overline{h(t)} + \frac{1}{2} u_t k(t). \quad (69)$$

The conservation of the energy $\mathcal{E}(\phi_t, \gamma_t, \sigma_t)$ follows.

Proof. Equation (58) is equivalent to

$$\begin{aligned} \gamma_t &= u_t^* \gamma'_0 u_t + v_t^T (1 + \bar{\gamma}'_0) \bar{v}_t, \\ \sigma_t &= u_t^* \gamma'_0 v_t + v_t^T (1 + \bar{\gamma}'_0) \bar{u}_t. \end{aligned}$$

Hence, we can rewrite the expression of the energy in terms of ϕ_t , u_t , and v_t as $\mathcal{E}(\phi_t, \gamma_t, \sigma_t) = \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t)$. We then compute the derivatives of $\mathcal{H}_{\gamma'_0}$:

$$\begin{aligned}\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \bar{\phi}}(\phi, u, v) &= h\phi + b[u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v}] \phi + k[\sigma + \phi \otimes \phi] \bar{\phi}, \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi, u, v) &= \gamma'_0 u (h + b[|\phi\rangle\langle\phi|] + b[u^* \gamma'_0 u + v^T (1 + \bar{\gamma}'_0) \bar{v}]) \\ &\quad + \left(\frac{1}{2} + \gamma'_0\right) v k[v^* \gamma'_0 u + u^T (1 + \bar{\gamma}'_0) \bar{v} + |\bar{\phi}\rangle\langle\phi|], \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi, u, v) &= (1 + \gamma'_0) v (\bar{h} + b[|\bar{\phi}\rangle\langle\bar{\phi}|] + b[u^T \bar{\gamma}'_0 \bar{u} + v^* (1 + \gamma'_0) v]) \\ &\quad + \left(\frac{1}{2} + \gamma'_0\right) u k[u^* \gamma'_0 v + v^T (1 + \bar{\gamma}'_0) \bar{u} + |\phi\rangle\langle\bar{\phi}|].\end{aligned}$$

Replacing (ϕ, u, v) by (ϕ_t, u_t, v_t) yields

$$\begin{aligned}\frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \bar{\phi}}(\phi_t, u_t, v_t) &= h\phi_t + b[\gamma_t] \phi_t + k(t) \bar{\phi}_t, \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi_t, u_t, v_t) &= \gamma'_0 u_t h(t) + \left(\frac{1}{2} + \gamma'_0\right) v_t \overline{k(t)}, \\ \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi_t, u_t, v_t) &= (1 + \gamma'_0) v_t \overline{h(t)} + \left(\frac{1}{2} + \gamma'_0\right) u_t k(t),\end{aligned}$$

which are in fact (67), (68), (69) using the HFB equations. Hence, using first the chain rule, then (67), (68), and (69),

$$\begin{aligned}\frac{d}{dt} \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t) &= \langle \partial_t \phi_t | \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial \langle \phi |}(\phi_t, u_t, v_t) + \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial |\phi\rangle}(\phi_t, u_t, v_t) | \partial_t \phi_t \rangle \\ &\quad + \text{Tr}[\partial_t u_t^* \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u^*}(\phi_t, u_t, v_t)] + \text{Tr}[\partial_t u_t \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial u}(\phi_t, u_t, v_t)] \\ &\quad + \text{Tr}[\partial_t v_t^* \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v^*}(\phi_t, u_t, v_t)] + \text{Tr}[\partial_t v_t \frac{\partial \mathcal{H}_{\gamma'_0}}{\partial v}(\phi_t, u_t, v_t)] \\ &= \text{Re Tr}[\partial_t u_t^* v_t \overline{k(t)} + \partial_t v_t^* (v_t \overline{h(t)} + \frac{1}{2} u_t k(t))].\end{aligned}$$

We can now use that the evolution Eq. (57) on $\mathcal{U}_t$ is equivalent to

$$i \partial_t u_t = u_t h(t) + v_t \overline{k(t)}, \quad (70)$$

$$i \partial_t v_t = -u_t k(t) - v_t \overline{h(t)}, \quad (71)$$

along with $\text{Tr}[A^T] = \text{Tr}[A]$ and the cyclicity of trace to group all the terms as in

$$\begin{aligned}\frac{d}{dt} \mathcal{H}_{\gamma'_0}(\phi_t, u_t, v_t) &= \text{Im Tr}[\overline{k(t)} h(t) (v_t^T \bar{u}_t - u_t^* v_t) - \overline{k(t)} k(t) v_t^* v_t \\ &\quad + \overline{k(t)} h(t) v_t^T \bar{u}_t + 2h(t) h(t) v_t^T \bar{v}_t + \overline{k(t)} k(t) u_t^T \bar{u}_t + h(t) k(t) u_t^T \bar{v}_t]\end{aligned}$$

Table 1. Correspondence between the notations of this article and some notations common in the physics literature [21]

This article	$\phi(x)$	$\gamma(x; x)$	$\sigma(x, x)$	$h_{g\delta}$	$k_{g\delta}$	N_j	V
[21]	$\Phi(\mathbf{r})$	$\tilde{n}(\mathbf{r})$	$\tilde{m}(\mathbf{r})$	$\hat{\mathcal{L}}$	$gm(\mathbf{r})$	$N_0(E_j)$	$U_{ext} - \mu$

which then vanishes since $v_t^T \bar{u}_t = u_t^* v_t$ for a symplectomorphism (see (55)), and the terms $\overline{k(t)}k(t)v_t^* v_t$, $h(t)h(t)v_t^T \bar{v}_t$, $\overline{k(t)}k(t)u_t^T \bar{u}_t$, and $\overline{k(t)}h(t)v_t^T \bar{u}_t + h(t)k(t)u_t^T \bar{v}_t$ give real traces. $\square$

Relation to the HFB eigenvalue equations. Now, we link our work with the HFB eigenvalue equations often encountered in the physics literature [19, 21, 42].

To be explicit, we give, in Table 1, the correspondence between the notations of this article and those of an article of Griffin [21].

We note that the setting in [21] is not exactly the same as ours, since the class of external potentials V that we consider excludes trapping potentials, and the solutions $\Phi(\mathbf{r})$ considered in [21] are time-independent. Moreover, we note that in this paper, we give rigorous proofs in the case of a two-body interaction potential v such that v^2 is relatively form-bounded with respect to the Laplacian, which excludes potentials as singular as $g\delta$; hence, the correspondence we establish in this section is only formal. Nevertheless, we believe that pointing out this relationship is useful.

Moreover, we note that in the physics literature (see, e.g., [21, (23)]), the HFB eigenvalue equations are often investigated using a generalized eigenbasis decomposition (using vectors often denoted by u_j , v_j which play the same role as below), which we can relate to our approach in the following manner, based on our discussion from Sect. 3.

Let $\mathcal{U}_t = \begin{pmatrix} u_t & v_t \\ \bar{u}_t & \bar{v}_t \end{pmatrix}$, and let $\gamma'_0 \geq 0$ be a trace class operator as in Prop. 3.9, with the orthonormal decomposition $\gamma'_0 = \sum_{j \geq 0} N_j |\zeta_j\rangle\langle\zeta_j|$. Let

$$u_{j,t} := u_t^* \zeta_j \quad \text{and} \quad v_{j,t} := -v_t^* \zeta_j.$$

Then, (58) yields

$$\begin{aligned} \gamma_t &= \sum_{j \geq 0} (N_j |u_{j,t}\rangle\langle u_{j,t}| + (1 + N_j) |\bar{v}_{j,t}\rangle\langle \bar{v}_{j,t}|), \\ \sigma_t &= \sum_{j \geq 0} (N_j |u_{j,t}\rangle\langle v_{j,t}| + (1 + N_j) |\bar{v}_{j,t}\rangle\langle \bar{u}_{j,t}|). \end{aligned}$$

which yield [21, (25)] by evaluation on the diagonal:

$$\gamma_t(x; x) = \sum_{j \geq 0} (N_j |u_{j,t}(x)|^2 + (1 + N_j) |\bar{v}_{j,t}(x)|^2), \quad (72)$$

$$\sigma_t(x, x) = \sum_{j \geq 0} u_{j,t}(x) \bar{v}_{j,t}(x) (1 + 2N_j). \quad (73)$$

We now consider a pair interaction potential $v = g\delta$. We assume that ϕ is independent of time and $u_{j,t}, v_{j,t}$ have the simple form:

$$u_{j,t} = e^{-itE_j} u_{j,0}, \quad v_{j,t} = e^{-itE_j} v_{j,0}. \quad (74)$$

We also distinguish the quantities corresponding to $v = g\delta$ by the index $g\delta$. Then, (57) formally yields the HFB eigenvalue equations:

$$\begin{aligned} h_{g\delta} u_j - k_{g\delta} v_j &= E_j u_j, \\ \overline{h_{g\delta}} v_j - \overline{k_{g\delta}} u_j &= -E_j v_j, \end{aligned}$$

as presented in the work of Griffin [21, Eq. (23)]. Note that (72), (73), and (74) imply that $\gamma_t(x; x)$ and $\sigma_t(x; x)$ are time independent, since the phases simplify.

We conclude that the HFB eigenvalue equations are the stationary version of our Eq. (57). It amounts to finding eigenvalues and eigenvectors for the matrix ΛS in (57), which is a nonlinear problem since Λ depends on γ and σ (that is, on u, v and γ'_0). Furthermore, the decomposition in functions u_j and v_j corresponds to a “diagonalization” of the generalized one-particle density matrix Γ in the sense of Proposition 3.8.

4. Existence and uniqueness of solutions to the HFB equations

We prove the global in time existence and uniqueness of mild solutions to the time-dependent Hartree–Fock–Bogoliubov equations in the H^1 -setting.

We recall that, given a Banach space X , $f \in C(X)$, a continuous function on X , and $-iA$ the infinitesimal generator of a strongly continuous semigroup $G(t)$ on X , a continuous function $\rho : [0, T) \rightarrow X$ is called a *mild solution* of the problem

$$\begin{cases} i\partial_t \rho &= A\rho + f(\rho), \\ \rho(0) &= \rho_0 \in X, \end{cases} \quad (75)$$

if ρ_t solves the fixed point equation in integral form (with the integral in Bochner’s sense)

$$\rho_t = G(t)\rho_0 - i \int_0^t G(t-s) f(\rho_s) ds. \quad (76)$$

In what follows we use the notation $A \lesssim B$ to stand for an inequality of the form $A \leq CB$, for some constant where $C > 0$. The main result of this section is the following

Theorem 4.1. *Let $d \leq 3$ and $\rho_0 = (\phi_0, \gamma_0, \sigma_0) \in X^1$. Assume that the potentials V and v satisfy Conditions (a) and (b’) of Sect. 1.1. Then the following hold:*

(i) *Existence and uniqueness of a local mild solution:*

There exists a unique maximal solution

$$(\rho_t)_{t \in [0, T]} = (\phi_t, \gamma_t, \sigma_t)_{t \in [0, T]} \in C^0([0, T]; X^1)$$

to the HBF Eqs. (39) to (41) in the mild sense, for some $0 < T \leq \infty$.

(ii) *Existence and uniqueness of a local classical solution:*

If $\rho_0 \in X^3$, then

$$(\rho_t)_{t \in [0, T]} \in C^0([0, T]; X^3) \cap C^1([0, T]; X^1)$$

and ρ_t satisfies the HBF Eqs. (39) to (41) in the classical sense.

(iii) *Conservation laws:*

The number of particles $\text{Tr}[\gamma_t]$ and the energy (47) are constants.

(iv) *Positivity preservation property:*

If $\Gamma = \begin{pmatrix} \gamma & \sigma \\ \bar{\sigma} & 1 + \bar{\gamma} \end{pmatrix} \geq 0$ at $t = 0$, then this holds for all times.

(v) *Existence of a global solution:*

If additionally $\Gamma_0 \geq 0$, then the solution ρ_t is global, i.e., $T = \infty$.

Proof of Theorem 4.1(i) [Local Mild Solutions] We use the notations introduced at the beginning of Sect. 2. The proof is based on a standard fixed point argument (through an application of the Cauchy–Lipschitz and Picard–Lindelöf theorem). Separating the linear part $A\rho$ and nonlinear part $f(\rho)$, we can write the HFB Eqs. (39) to (41) in the form:

$$i \partial_t \rho = A\rho + f(\rho), \quad (77)$$

where $\rho := (\phi, \gamma, \sigma) \in X^2$. Then, the linear part in the HFB equations is given by

$$A\rho = (h\phi, [h, \gamma], [h, \sigma]_+ + k[\sigma]), \quad (78)$$

with the domain $D(A) = X^2$, and the nonlinear part $f := (f_1, f_2, f_3)$ by

$$f_1(\rho) = b[\gamma]\phi + k[\sigma + \phi^{\otimes 2}]\bar{\phi}, \quad (79)$$

$$f_2(\rho) = [b[\gamma + |\phi\rangle\langle\phi|], \gamma] + k[\sigma + \phi^{\otimes 2}]\bar{\sigma} - \overline{\sigma k[\sigma + \phi^{\otimes 2}]}, \quad (80)$$

$$f_3(\rho) = [b[\gamma + |\phi\rangle\langle\phi|], \sigma]_+ + [k[\sigma + \phi^{\otimes 2}], \gamma]_+. \quad (81)$$

From Lemma 4.3, below, we obtain that f is continuously Fréchet differentiable in X^1 and therefore is locally Lipschitz, and from Lemma 4.2, we obtain that $G(t) = \exp(itA)$ defines a strongly continuous uniformly bounded semigroup on X^1 .

Consequently, we can rewrite the HFB Eqs. (39)–(41) as a fixed point problem

$$\rho_t = G(t)\rho_0 - i \int_0^t G(t-s)f(\rho_s) ds.$$

and use the Banach contraction theorem to show that (39)–(41) have the unique local mild solution to in X^1 for the given initial data. (For the details for this standard argument, see [34, Sect. 9.2e, Thm 3].) $\square$

We will now prove our main Lemmata on $G(t) = \exp(itA)$ and f . First, we recall the norms (37). Moreover, if we denote the integral kernel of an operator σ by $\tilde{\sigma}$, then the norm $\|\sigma\|_{\mathcal{H}_\sigma^j}$ is equivalent to the norm

$$\|\sigma\|_{\mathcal{H}_\sigma^j} \simeq \|\tilde{\sigma}\|_{H^j} := \|(M^2 \otimes 1 + 1 \otimes M^2)^{j/2} \tilde{\sigma}\|_{L^2(\mathbb{R}^{2d})}.$$

Lemma 4.2. *The operator A generates a strongly continuous semigroup, $G(t) = \exp(itA)$, on X^1 , uniformly bounded as $\|G(t)\|_{\mathcal{B}(X^1)} \leq 1$.*

Proof. Let $\hat{h}(\sigma) := [h, \sigma]_+ + k[\sigma]$. We define $G(t) = \exp(itA)$ on $\rho := (\phi, \gamma, \sigma) \in X^j$ as

$$G(t)\rho := (\exp(-ith)\phi, \exp(-ith)\gamma \exp(ith), \exp(-it\hat{h})(\sigma)). \quad (82)$$

We use that $-\Delta$ is h -bounded, and h is $-\Delta$ -bounded and that M is translationally invariant. For $(\phi, \gamma, \sigma) \in X^1$ and $C < \infty$ chosen s.t. $M \leq h + C$,

$$\|\exp(-ith)\phi\|_{H^1} = \|(h + C)\exp(-ith)\phi\|_{L^2} = \|(h + C)\phi\|_{L^2}^2 \lesssim \|\phi\|_{H^1}.$$

Similarly $\|\exp(-ith)\gamma \exp(ith)\|_{\mathcal{H}_\gamma^1} \lesssim \|\gamma\|_{\mathcal{H}_\gamma^1}$.

Finally, we define the operator $\tilde{h}$ acting on $L^2(\mathbb{R}^{2d})$ by the condition $\widetilde{\hat{h}(\sigma)} = \tilde{h}\tilde{\sigma}$. Then, we have $\tilde{h} = h_x + h_y + v(x - y)$, since the pair potential v be infinitesimally bounded with respect to $-\Delta$, the operator $\tilde{h} = h_x + h_y + v(x - y)$ is self-adjoint and h and $-\Delta_x - \Delta_y$ are mutually relatively bounded. Hence, using (82) and choosing c s.t. $M_x + M_y \leq \tilde{h} + c$,

$$\begin{aligned} \|\exp(-it([h, \sigma]_+ + k[\sigma]))\sigma\|_{\mathcal{H}_\sigma^1} &\simeq \|\exp(-it\tilde{h})\tilde{\sigma}\|_{H^1} \\ &\lesssim \|(\tilde{h} + c)\exp(-it\tilde{h})\tilde{\sigma}\|_{L^2} \lesssim \|\tilde{\sigma}\|_{H^1} \simeq \|\sigma\|_{\mathcal{H}_\sigma^1}. \end{aligned}$$

The strong continuity of $G(t)$ follows from the strong continuity of $\exp(-ith)$ and $\exp(-it\hat{h})$. $\square$

The following lemma allows us to control the nonlinear term f in the HFB equations.

Lemma 4.3. *The vector of nonlinear terms $f = (f_1, f_2, f_3)$ defined in Eq. (79)–(81) maps X^1 into itself and is continuously Fréchet differentiable in X^1 ($f \in C^1(X^1)$).*

Proof of Lemma 4.3. For the first statement, it is sufficient to prove that, for the quadratic and cubic parts of f are bounded as:

$$\begin{aligned} &\|(b[\gamma]\phi + k[\sigma]\bar{\phi}, [b[\gamma], \gamma] + k[\sigma]\bar{\sigma} - \sigma\overline{k[\sigma]}, [b[\gamma], \sigma]_+ + [k[\sigma], \gamma]_+)\|_{X^1} \\ &\lesssim \|\rho\|_{X^1}^2, \end{aligned} \quad (83)$$

$$\begin{aligned} &\|(k[\phi^{\otimes 2}]\bar{\phi}, [b[|\phi\rangle\langle\phi|], \gamma] + k[\phi^{\otimes 2}]\bar{\sigma} - \sigma\overline{k[\phi^{\otimes 2}]}, \\ &\quad [b[|\phi\rangle\langle\phi|], \sigma]_+ + [k[\phi^{\otimes 2}], \gamma]_+)\|_{X^1} \lesssim \|\rho\|_{X^1}^3. \end{aligned} \quad (84)$$

All the cubic estimates can be deduced from their quadratic counterparts using

$$\|\phi\|\langle\phi\|\|_{\mathcal{H}_\gamma^1} \leq \|\phi\|_{H^1}^2 \quad \text{and} \quad \|\phi \otimes \phi\|_{H^1} \leq \|\phi\|_{H^1}^2.$$

We thus only consider the quadratic terms. Using Lemma 4.5 (i), we estimate

$$\|b[\gamma]\phi\|_{H^1} \lesssim \|\gamma\|_{\mathcal{H}_\gamma^1} \|\phi\|_{H^1} \lesssim \|\rho\|_{X^1}^2.$$

For $k[\sigma]\bar{\phi}$, we use Lemma 4.5 (ii) to find

$$\|k[\sigma]\bar{\phi}\|_{H^1} \leq \|Mk[\sigma]\|_{\mathcal{B}} \|\bar{\phi}\|_{L^2} \lesssim \|\sigma\|_{\mathcal{H}_\sigma^1} \|\phi\|_{L^2}.$$

We estimate $[b[\gamma], \gamma]$ using Lemma 4.5 (i),

$$\begin{aligned} \|[b[\gamma], \gamma]\|_{\mathcal{H}_\gamma^1} &\leq 2\|Mb[\gamma]M^{-1}M\gamma M\|_{\mathcal{L}^1} \\ &\leq 2\|b[\gamma]\|_{\mathcal{H}_\gamma^1} \|\gamma\|_{\mathcal{H}_\gamma^1} \lesssim \|\gamma\|_{\mathcal{H}_\gamma^1}^2 \lesssim \|\rho\|_{X^1}^2. \end{aligned}$$

For $k[\sigma]\bar{\sigma}$ (and similarly $\sigma\overline{k[\sigma]}$), the inequality

$$\|k[\sigma]\bar{\sigma}\|_{\mathcal{H}_\gamma^1} = \|Mk[\sigma]\bar{\sigma}M\|_{\mathcal{L}^1} \leq \|Mk[\sigma]\|_{\mathcal{L}^2} \|\bar{\sigma}M\|_{\mathcal{L}^2},$$

Lemma 4.5 (ii) (see estimate (95))

and $\|\bar{\sigma}M\|_{\mathcal{L}^2} \leq \|\sigma\|_{\mathcal{H}_\sigma^1}$ (which follows from the definition of $\|\sigma\|_{\mathcal{H}_\sigma^1}$) give the estimate

$$\|k[\sigma]\bar{\sigma}\|_{\mathcal{H}_\gamma^1} \lesssim \|\sigma\|_{\mathcal{H}_\sigma^1}^2. \quad (85)$$

For $b[\gamma]\sigma$ (or similarly $\sigma\overline{b[\gamma]}$), using Lemma 4.5 (i), we obtain

$$\|b[\gamma]\sigma\|_{\mathcal{H}_\sigma^1} \leq \|Mb[\gamma]M^{-1}\|_{\mathcal{B}} \|M\sigma M\|_{\mathcal{L}^2} \lesssim \|\gamma\|_{\mathcal{H}_\gamma^1} \|\sigma\|_{\mathcal{H}_\sigma^1}.$$

And finally $k[\sigma]\bar{\gamma}$ (and similarly $\gamma\overline{k[\sigma]}$), using Lemma 4.5 (ii) (see estimate (95)), we arrive at

$$\|k[\sigma]\bar{\gamma}\|_{\mathcal{H}_\sigma^1} \leq \|Mk[\sigma]\|_{\mathcal{L}^2} \|\bar{\gamma}M\|_{\mathcal{B}} \lesssim \|\sigma\|_{\mathcal{H}_\sigma^1} \|\gamma\|_{\mathcal{H}_\gamma^1},$$

which completes the proof of (83) and therefore of (84).

To prove that f is Fréchet differentiable, we observe that each f_j is a linear combination of multi-linear maps and therefore $df(\rho)\xi$ is of the same form as $f(\rho)$ and can be estimated as above. $\square$

Proof of Theorem 4.1(ii) [Local Classical Solutions] The existence of classical solutions to the HFB equations for initial data in X^3 then follows from: $\square$

Lemma 4.4 (See [46, Lemma 3.1]). *If $-iA$ is the generator of a continuous one-parameter semi-group in the Banach space X , and if f is continuously differentiable on X , then a mild solution of Eq. (75) has its values in the domain $\mathcal{D}(A)$ of A throughout its interval of existence provided this is the case initially.*

In other words, ρ_t , if it exists at all, then satisfies the differential Eq. (75) in the obvious sense. $\square$

Proof of Theorem 4.1(iii) [Conservation Laws] For classical solutions, the conservation of the number particle and of the energy were proven as a consequence of the same conservation laws for the many-body system in Theorem 2.6 and 2.4. Another proof of the conservation law for the energy using only the HFB equations (independently from the many body problem) was given in Prop. 3.12, and the conservation of the particle number could also be proven directly from (40). We can now use those results since we proved the local existence of a classical solution. The conservation laws then extend to mild solutions by approximation. $\square$

Proof of Theorem 4.1(iv) [Positivity preservation property]

This follows from relation (62). Indirectly, it follows from the equivalence of the HFB Eqs. (39) to (41) the self-consistent Eq. (45) (see Theorem 2.3). $\square$

Proof of Theorem 4.1(v) [Global Solution] We recall that for a maximal solution ρ_t of the mild problem (76) defined on an interval $[0, T)$, we have that either $T = \infty$ or $\sup_{t \in [0, T)} \|\rho_t\|_{X^1} = \infty$ (see, e.g., [14, Thm 4.3.4]). It is thus enough to prove that

$$\sup_{t \in [0, T)} \{ \|\phi_t\|_{H^1}, \|\gamma_t\|_{\mathcal{H}_V^1}, \|\sigma_t\|_{\mathcal{H}_\sigma^1} \} < \infty$$

to show that the solutions are global. Let

$$\mathbb{T} := \int dx dy \psi^*(x) (-\Delta) \psi(y), \quad (86)$$

Because V is infinitesimally form bounded with respect to the Laplacian,

$$\int dx \psi^*(x) \psi(x) V(x) \geq -\frac{1}{2} \mathbb{T} - cN \quad (87)$$

holds. And, because the pair potential v is bounded, we have

$$\mathbb{V} := \frac{1}{2} \int dx dy v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y) \geq -CN^2 - CN. \quad (88)$$

Hence, from the definition of $\mathbb{H}$, (87) and (88) we get

$$\mathbb{T} \leq 2\mathbb{H} + CN^2 + CN. \quad (89)$$

We now take the expectation value of ω_t^q and use that ω_t^q is quasifree to bound $\omega_t^q(\mathbb{N}^2)$ by $C(\omega_t^q(\mathbb{N})^2 + 1)$ and the conservation of the particle number and of the energy to obtain

$$\begin{aligned} \text{Tr}[-\Delta(\gamma_t + |\phi_t\rangle\langle\phi_t|)] &\leq C(\mathcal{E}(\phi_t, \gamma_t, \sigma_t) + \sum_{k=0}^2 \mathcal{N}(\phi_t, \gamma_t, \sigma_t)^k) \\ &\leq C(\mathcal{E}(\phi_0, \gamma_0, \sigma_0) + \sum_{k=0}^2 \mathcal{N}(\phi_0, \gamma_0, \sigma_0)^k). \end{aligned} \quad (90)$$

Combined with the conservation of the particle number, this estimate provides bounds on $\|\gamma_t\|_{\mathcal{H}_\gamma^1}$ and $\|\phi_t\|_{H^1}$ that are uniform in t . Moreover, uniform bounds on $\|\sigma_t\|_{\mathcal{H}_\sigma^1}$ are then obtained from Proposition 3.1. It thus follows that the solution is global, as claimed. $\square$

Recall that $W^{p,r}(\mathbb{R}^d)$ denotes the standard Sobolev space over $\mathbb{R}^d$.

Lemma 4.5. *Assume that $v \in W^{p,1}$ with $p > d$. Then, the operators b and k defined in (42) and (43) possess the following properties:*

- (i) *b is continuous from $\mathcal{H}_\gamma^1$ to $\mathcal{B}(H^1) \simeq MBM^{-1}$.*
- (ii) *k is continuous from $\mathcal{H}_\sigma^1$ to $M^{-1}\mathcal{L}^2$.*

Proof. For the detailed proof of statement (i), we refer to [12]. For the reader's convenience, we recall here the main arguments. We first consider the direct term, i.e., the first term in the definition of b . It is sufficient to prove that $v * n$ (with functions $n(x) = \gamma(x; x)$) and $\nabla v * n$ uniformly bounded by $\|\gamma\|_{\mathcal{H}_\gamma^1}$. As those two bounds are very similar, we focus on the more difficult one, $\nabla v * n$.

Denote by $\tilde{\gamma}$ the (generalized) integral kernel of an operator γ . Since $v \in W^{p,1}(\mathbb{R}^d)$ with $p > d$, the function v is bounded. Since $\nabla_x \int_{\mathbb{R}^d} v(x-y) \gamma(y; y) dy = \int_{\mathbb{R}^d} v(x-y) \nabla_y \gamma(y; y) dy$, we have

$$\left\| \nabla_x \int_{\mathbb{R}^d} v(x-y) \gamma(y; y) dy \right\|_\infty \leq \|v\|_\infty \int_{\mathbb{R}^d} |\nabla_y \gamma(y; y)| dy \quad (91)$$

Furthermore, $\int_{\mathbb{R}^d} |\nabla_y \gamma(y; y)| dy \leq \|\gamma\|_{\mathcal{H}_\gamma^1}$, which can be proved by using the decomposition $\gamma = \sum_{j=1}^\infty \lambda_j |\varphi_j\rangle\langle\varphi_j|$ with $\lambda_j \geq 0$ of γ , combined with the Cauchy–Schwarz inequality:

$$\int_{\mathbb{R}^d} |\nabla_y \gamma(y; y)| dy \leq \sum_{j=1}^\infty \lambda_j \int_{\mathbb{R}^d} |\varphi_j(y) \nabla \varphi_j(y)| dy \quad (92)$$

$$\leq \sum_{j=1}^\infty \lambda_j \|\varphi_j\|_{L^2} \|\nabla \varphi_j\|_{L^2} \quad (93)$$

$$\leq \sum_{j=1}^\infty \lambda_j \|M\varphi_j\|_{L^2}^2 \leq \|\gamma\|_{\mathcal{H}_\gamma^1} \quad (94)$$

The last two estimates imply the desired result, $\|\nabla v * n\|_\infty \leq \|\gamma\|_{\mathcal{H}_\gamma^1}$. The estimates for the exchange term (the second term in the definition of B) are similar.

Point (ii) is equivalent to the estimate

$$\|Mk[\sigma]\|_{\mathcal{L}^2} \lesssim \|\sigma\|_{\mathcal{H}_\sigma^1}, \quad (95)$$

which we now prove.

Denote by $\tilde{\sigma}$ the (generalized) integral kernel of an operator σ . Clearly, $\|\sigma\|_{\mathcal{H}_\sigma^1} \simeq \|\tilde{\sigma}\|_{H^1}$. Denote by $a(x, y) = v(x-y)\tilde{\sigma}(x, y)$, the integral kernel of $k[\sigma]$. We have

that

$$\|Mk\|_{L^2}^2 = \int \int |M_x a(x, y)|^2 dx dy \leq \|a\|_{H^1}^2. \quad (96)$$

Since $a(x, y) = v(x - y)\tilde{\sigma}(x, y)$ and

$$\|a\|_{H^1} \leq \|a\|_{L^2} + \|\partial_x a\|_{L^2} + \|\partial_y a\|_{L^2},$$

we use the Leibniz rule, $\partial_x a(x, y) = (\partial v(x - y))\tilde{\sigma}(x, y) + v(x - y)\partial_x \tilde{\sigma}(x, y)$, to find that

$$\|a\|_{H^1} \leq (\|v\|_{L^\infty} + \|\partial_x v M_x^{-1}\|_{B(L^2)} + \|\partial_y v M_y^{-1}\|_{B(L^2)}) \|\tilde{\sigma}\|_{H^1}, \quad (97)$$

where $L^2 := L^2(\mathbb{R}_x^d \times \mathbb{R}_y^d)$. The Schwartz and Sobolev inequalities imply that

$$\|\partial_x v f\|_{L^2} \leq \|\partial_x v\|_{L^p} \|f\|_{L^s} \lesssim \|v\|_{W^{p,1}} \|Mf\|_{L^2},$$

for arbitrary s and p satisfying $\frac{1}{p} + \frac{1}{s} = \frac{1}{2}$ and $p > d$. Thus,

$$\|\partial_x v M_x^{-1}\| \lesssim \|v\|_{W^{p,1}},$$

and, similarly, $\|\partial_y v M_y^{-1}\| \lesssim \|v\|_{W^{p,1}}$. It follows that

$$\|a\|_{H^1} \lesssim \|v\|_{W^{p,1}} \|\tilde{\sigma}\|_{H^1}. \quad (98)$$

This, together with (96) and $\|\tilde{\sigma}\|_{H^1} \simeq \|\sigma\|_{\mathcal{H}_d^1}$, yields (95). $\square$

5. Gibbs states and Bose–Einstein condensation

In this section, we determine translation- and $U(1)$ gauge-invariant Gibbs states for the HFB equations without an external potential, and with an interaction potential $g\delta$, and discuss the emergence of a Bose–Einstein condensate at positive temperature. (Recall from the introduction that $U(1)$ gauge-invariant Gibbs states for the HFB equations are, in fact, Gibbs states for the Hartree-Fock equations.)

We consider the system on a torus, $\Lambda_L = \mathbb{R}^d/2L\mathbb{Z}^d$, i.e., $[-L, L]^d$ with periodic boundary conditions. Accordingly, we denote $\Lambda_L^* := \frac{\pi}{L}\mathbb{Z}^d$ the lattice reciprocal to $2L\mathbb{Z}^d$. We will eventually take the thermodynamic limit, $L \rightarrow \infty$, and discuss the emergence of a Bose–Einstein condensate.

The Hamiltonian $\mathbb{H}$ of the Bose gas is $U(1)$ gauge-invariant (that is, invariant under the transformation $\psi^\sharp \rightarrow (e^{i\theta}\psi)^\sharp$), and, as we consider the case with no external potential, translation invariant. On a compact torus, where the volume is finite, these symmetries are also present in the Gibbs states of system (the notion of translation invariance should be, of course, appropriately modified). We are interested in quasifree

states ω_L^q which, on the one hand, satisfy both the $U(1)$ gauge invariance and the translation invariance, and, on the other hand, satisfy a fixed point equation corresponding to the consistency condition (45) in the dynamical case:

$$\Phi(\omega_L^q) = \omega_L^q \quad \text{with} \quad \Phi(\omega_L^q)(\mathbb{A}) := \text{Tr}[\mathbb{A} \exp(-\beta(\mathbb{H}_{HFB}(\omega_L^q) - \mu\mathbb{N}))/\Xi] \quad (99)$$

where $\beta > 0$ is the inverse temperature, μ is the chemical potential, and $\Xi = \text{Tr}[\exp(-\beta(\mathbb{H}_{HFB}(\omega_L^q) - \mu\mathbb{N}))]$. The $U(1)$ gauge-invariance of ω_L^q then implies that the truncated expectations $\phi_{\omega_L^q}$ and $\sigma_{\omega_L^q}$ vanish. Indeed, if one of them was nonzero, then the HFB Hamiltonian $\mathbb{H}_{HFB}$ would include terms which would break $U(1)$ gauge invariance, such as $\int dx \, m(x) \psi^*(x) \psi(x) + h.c.$. The quasifree states we consider are thus characterized by their truncated expectation γ_L , and we will replace the variable ω_L^q by γ_L in the sequel of this section.

We use the expression of the HFB Hamiltonian (44) with $v = g\delta$ (and $\phi = 0, \sigma = 0$), although this expression was derived for more regular interaction potentials v 's:

$$\mathbb{H}_{HFB}(\omega_L^q) = \int dx dy \, \psi^*(x) \psi(y) (-\Delta + gn)(x; y), \quad (100)$$

with $n = n(x) = \gamma_L(x; x)$. The translation invariance implies that the kernel $\gamma_L(x; y)$ is a function of $x - y$, that we still denote by γ_L , and therefore $n = n(x) = \gamma_L(x; x)$ is independent of x .

Applying the fixed point Eq. (99) with $\mathbb{A} = \psi^*(y) \psi(x)$, one can express it equivalently in the variable γ_L :

$$\gamma_L = \frac{1}{\exp(\beta(-\Delta + gn\mathbf{1} - \mu\mathbf{1})) - \mathbf{1}}, \quad (101)$$

for $n \in [0, \infty)$. The operator γ_L is a pseudodifferential operator with symbol

$$\hat{\gamma}_L(k) := \int_{\Lambda_L} \gamma_L(x) e^{-ix \cdot k} dx = \frac{1}{\exp(\beta(k^2 + gn - \mu)) - 1} \quad (102)$$

of γ_L . Thus,

$$n = \gamma_L(0) = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k). \quad (103)$$

As the Fourier coefficients of γ_L depend only of the number n , we obtain from (101), (102) and (103) a *nonlinear fixed point equation* for n :

$$n = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{1}{\exp(\beta(k^2 + gn - \mu)) - 1}. \quad (104)$$

Note that the knowledge of n satisfying (104), or of γ_L satisfying (101) or of ω_L^q satisfying (99) are equivalent.

From a physical point of view, it is natural to fix the density n , which can be tuned in an experiment and to compute μ . So n is a parameter and we solve (104) with the unknown μ .

Lemma 5.1. *Let $g, \beta, n > 0$, and, for $d \geq 3$. Let n_c be the critical density*

$$n_c := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{dk}{e^{\beta k^2} - 1} = \frac{\zeta(\frac{d}{2})\Gamma(\frac{d}{2})}{(2\pi)^d} \beta^{-\frac{d}{2}}, \quad (105)$$

where $\zeta(x) = \sum_{n \geq 1} n^{-x}$ and $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$.

We define $S_L : (-\infty, gn) \rightarrow \mathbb{R}$ and $S_\infty : (-\infty, gn] \rightarrow \mathbb{R}$ through

$$S_L(\mu) := \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{1}{\exp(\beta(k^2 + gn - \mu)) - 1},$$

$$S_\infty(\mu) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \frac{dk}{\exp(\beta(k^2 + gn - \mu)) - 1}.$$

Then:

- There exists a unique $\mu_L(n) < gn$ such that (104) holds, i.e.,

$$n = S_L(\mu_L(n)). \quad (106)$$

- If $n < n_c$, there exists a unique $\mu_\infty(n) < gn$ such that

$$n = S_\infty(\mu_\infty(n)). \quad (107)$$

We extend the function μ_∞ to $(0, \infty)$ by setting $\mu_\infty(n) = gn$ for $n \geq n_c$.

Remark 5.2. The critical density n_c can be explicitly computed.

Proof. In the discrete case, the existence follows from the intermediate value theorem because the map S_L is continuous with limits 0 at $-\infty$ and ∞ at gn . The map S_L is strictly increasing and thus there exists a unique $\mu_L(n)$ such that $n = S_L(\mu_L(n))$.

In the continuous case, we first prove the existence of $\mu_\infty(n)$, for a given $n > 0$, the map $(0, gn] \ni \mu \mapsto S_\infty(\mu)$ is well-defined, continuous, $\lim_{\mu \rightarrow -\infty} S_\infty(\mu) = 0$, $S_\infty(gn) = n_c$, and thus the intermediate value theorem yields the existence of a μ_∞ satisfying (107). Since S_∞ is strictly increasing, the uniqueness follows. $\square$

In Theorem 5.3, we prove that the thermodynamic limit γ_∞ of the self-consistent Eq. (101) for γ_L is well-defined and exhibits the so-called Bose–Einstein condensation.

Theorem 5.3. *Let $g, \beta, n > 0$ and $d \geq 3$. Let γ_L, n_c, μ_L and μ_∞ as defined in (101) and Lemmata 5.1. Then,*

$$\mu_L(n) \xrightarrow{L \rightarrow \infty} \mu_\infty(n) \quad \text{and} \quad \gamma_L \xrightarrow{L \rightarrow \infty} \gamma_\infty, \quad (108)$$

where

$$\hat{\gamma}_\infty(k) = \max\{0, n - n_c\} \delta(k) + \frac{1}{\exp(\beta(k^2 + gn - \mu_\infty(n))) - 1}. \quad (109)$$

Remark 5.4. The presence of the $\delta(k)$ term is interpreted as the existence of Bose–Einstein condensation, because there is an accumulation of particles in the zero mode. It occurs when $\beta^{d/2}n \geq C_d$ with C_d a constant depending only on the dimension.

Proof of Theorem 5.3. First we prove the convergence of $\mu_L(n)$ towards a $\mu_\infty(n)$. We first remark that $\mu_L(n) \geq -C$ for some constant $C > 0$ independent of L . (Otherwise one could extract a subsequence such that $n = S_{L_j}(\mu_{L_j}(n)) \rightarrow 0 < n$.) Thus, the accumulation points of $\mu_L(n)$ are contained in $[-C, gn]$. Let $\mu_{L_j}(n)$ denote an extracted sequence converging to an accumulation point μ' .

In the case $n < n_c$: If $\mu' = gn$, then for j large enough $\mu_{L_j}(n) \geq (\mu_\infty(n) + gn)/2$, thus

$$n = S_{L_j}(\mu_{L_j}(n)) \geq S_{L_j}\left(\frac{gn + \mu_\infty(n)}{2}\right) \rightarrow S_\infty\left(\frac{gn + \mu_\infty(n)}{2}\right) > S_\infty(\mu_\infty(n)) = n$$

and which would lead to a contradiction. Note that it is crucial that $\mu_\infty(n) < gn$ for $n < n_c$ to get the convergence to the integral $S_\infty\left(\frac{gn + \mu_\infty(n)}{2}\right)$. It thus follows that $\mu' < gn$. Then $S_{L_j}(\mu_{L_j}(n))$ converges to n , because by definition of $\mu_L(n)$ this sum is equal to n , and also to $S_\infty(\mu')$. (One has to control the dependency in $\mu_{L_j}(n)$ in the Riemann sums.) Hence, $\mu' = \mu_\infty(n)$ and the unique accumulation point is $\mu_\infty(n)$. We thus proved the convergence of $\mu_L(n)$ to $\mu_\infty(n)$.

In the case $n \geq n_c$, we sketch an argument similar to the one above. If an accumulation point μ' was such that $\mu' < gn$, then the sums $S_{L_j}(\mu_{L_j}(n))$ would converge to integrals with a value strictly smaller than n_c and thus strictly smaller than n . This would lead to a contradiction. Thus, the only possible accumulation point is gn and $\mu_L(n) \rightarrow gn = \mu_\infty(n)$.

We now prove the convergence of γ_L towards γ_∞ . Let $\varphi \in C_0^\infty(\mathbb{R}^d)$. For L large enough the support of φ is included in Λ_L , and

$$\int_{\Lambda_L} \gamma_L \varphi = \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k) \hat{\varphi}(k). \quad (110)$$

On the other hand, $\langle \gamma_\infty, \varphi \rangle_{\mathcal{D}'} = \langle \gamma_\infty, \varphi \rangle_{S'} = \langle \hat{\gamma}_\infty, \hat{\varphi} \rangle_{S'}$ (Note that in the normalization we choose, the Fourier coefficients of φ on Λ_L and the Fourier transform coincide, there is thus no need to specify the hat notation.) The convergence of γ_L to γ_∞ is thus equivalent to

$$\frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \hat{\gamma}_L(k) \hat{\varphi}(k) \rightarrow \max\{0, n - n_c\} \hat{\varphi}(0) + \int_{\mathbb{R}^d} \frac{(2\pi)^{-d} \hat{\varphi}(k) dk}{e^{\beta(k^2 + gn - \mu_\infty(n))} - 1}. \quad (111)$$

for all φ .

In the case $n < n_c$ the convergence is thus just a convergence of Riemann sums of the integral (with the small additional difficulty that $\mu_L(n)$ depends on L in the sum) because there is no singularity in the function $k \mapsto (\exp(\beta(k^2 + gn - \mu_\infty(n))) - 1)^{-1}$.

In the case $n \geq n_c$: Let $\varepsilon > 0$. First note that, for any fixed $\eta > 0$

$$\frac{1}{|\Lambda_L|} \sum_{\substack{k \in \Lambda_L^* \\ |k| > \eta}} \frac{\hat{\varphi}(k)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} \rightarrow \int_{|k| > \eta} \frac{(2\pi)^{-d} \hat{\varphi}(k) dk}{e^{\beta k^2} - 1},$$

as $L \rightarrow \infty$. We choose $\eta > 0$ small enough so that

$$|k| \leq \eta \Rightarrow |\hat{\varphi}(k) - \hat{\varphi}(0)| \leq \frac{\varepsilon}{4n} \quad \text{and} \quad \int_{|k| \leq \eta} \frac{(2\pi)^{-d} \hat{\varphi}(0) dk}{e^{\beta k^2} - 1} \leq \frac{\varepsilon}{4}.$$

The first condition on η yields

$$\left| \frac{1}{|\Lambda_L|} \sum_{\substack{k \in \Lambda_L^* \\ |k| \leq \eta}} \frac{\hat{\varphi}(k) - \hat{\varphi}(0)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} \right| \leq \frac{\varepsilon}{4},$$

then, the second condition on η implies

$$\limsup_{L \rightarrow \infty} \left| \frac{1}{|\Lambda_L|} \sum_{\substack{k \in \Lambda_L^* \\ |k| \leq \eta}} \frac{\hat{\varphi}(0)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} - (n - n_c) \hat{\varphi}(0) \right| \leq \frac{\varepsilon}{4}.$$

Hence

$$\begin{aligned} \limsup_{L \rightarrow \infty} \left| \frac{1}{|\Lambda_L|} \sum_{k \in \Lambda_L^*} \frac{\hat{\varphi}(k)}{\exp(\beta(k^2 + gn - \mu_L(n))) - 1} \right. \\ \left. - (n - n_c) \hat{\varphi}(k) - \int_{\mathbb{R}^d} \frac{(2\pi)^{-d} \hat{\varphi}(k) dk}{e^{\beta k^2} - 1} \right| \leq \varepsilon, \end{aligned}$$

and as this holds for any $\varepsilon > 0$, we get the result. $\square$

6. Derivation of the Bosonic HFB equations

In this section, we prove Theorem 2.2. The derivations below are done in a somewhat informal way commonly used in dealing with operators on Fock spaces (see, e.g., [8, 13, 25]). For instance, the commutator $[A, H]$, for $A = \psi(x)$ and $A = \psi(x)\psi(y)$, contains the terms $\Delta_x \psi(x)$ and $\psi(x) \Delta_y \psi(y)$. The formal computation gives $\omega^q(\Delta_x \psi(x)) = \Delta_x \omega^q(\psi(x))$ and $\omega^q(\psi(x) \Delta_y \psi(y)) = \Delta_y \omega^q(\psi(x)\psi(y))$, which are well-defined by our assumptions and are equal to $\Delta_x \phi(x)$ and $\Delta_y \sigma(x, y)$, respectively.

To do this more carefully, one uses, instead of operator functions $\psi^\#(x)$, the operator functionals $\psi^\#(f)$, for some nice f . E.g., instead $[\psi(x), H]$, we consider the commutator $[\psi(f), H]$, for any nice f , and concentrate on the term $\psi(\Delta f)$ it contains. Clearly, ω^q is well-defined on $\psi(\Delta f)$ and can be written as $\omega^q(\psi(\Delta f)) = \int \Delta \bar{f}(x) \omega^q(\psi(x)) = \int \Delta \bar{f}(x) \phi(x) = \int \bar{f}(x) \Delta \phi(x)$. Thus, we obtain the same result as above but in a weak form.

Proof of Theorem 2.2. We first observe that the three following conditions are equivalent:

1. A quasifree state ω_t^q satisfies

$$i\partial_t\omega_t^q(\mathbb{A}) = \omega_t^q([\mathbb{A}, \mathbb{H}]), \quad (112)$$

for any operator $\mathbb{A}$ of order ≤ 2 in the fields.

2. A quasifree state ω_t^q satisfies

$$i\partial_t\omega_t^q(\psi(x)) = \omega_t^q([\psi(x), \mathbb{H}]), \quad (113)$$

$$i\partial_t\omega_t^q(\psi^*(y)\psi(x)) = \omega_t^q([\psi^*(y)\psi(x), \mathbb{H}]), \quad (114)$$

$$i\partial_t\omega_t^q(\psi(x)\psi(y)) = \omega_t^q([\psi(x)\psi(y), \mathbb{H}]). \quad (115)$$

3. A quasifree state ω_t^q with truncated expectations ϕ_t , γ_t and σ_t satisfies

$$i\partial_t\phi_t(x) = \omega_t^q([\psi(x), \mathbb{H}]), \quad (116)$$

$$i\partial_t\gamma_t(x; y) = \omega_t^q([\psi^*(y)\psi(x), \mathbb{H}]) - i\partial_t(\phi_t(x)\overline{\phi_t(y)}), \quad (117)$$

$$i\partial_t\sigma_t(x, y) = \omega_t^q([\psi(x)\psi(y), \mathbb{H}]) - i\partial_t(\phi_t(x)\phi_t(y)). \quad (118)$$

We now suppose ω_t^q satisfies (116)–(118). Using the definition of the Hamiltonian, we obtain

$$\begin{aligned} i\partial_t\phi_t(x) &= \omega_t^q\left([\psi(x), \int \psi^*(y)h(y; y')\psi(y') dy dy']\right) \\ &\quad + \frac{1}{2}[\psi(x), \int v(y - y')\psi^*(y)\psi^*(y')\psi(y')\psi(y) dy dy'] \end{aligned} \quad (119)$$

$$= \omega_t^q\left(\int h(x; y')\psi(y') dy' + \int v(x - y)\psi^*(y)\psi(y)\psi(x) dy\right), \quad (120)$$

where we used the CCR (3) to get

$$\begin{aligned} &[\psi(x), \psi^*(y)\psi^*(y')\psi(y')\psi(y)] \\ &= \delta(x - y)\psi^*(y')\psi(y')\psi(y) + \delta(x - y')\psi^*(y)\psi(y)\psi(y'). \end{aligned} \quad (121)$$

As ω_t^q is a quasifree state (see Appendix B)

$$\begin{aligned} \omega_t^q(\psi^*(y)\psi(y)\psi(x)) \\ = |\phi_t(y)|^2\phi_t(x) + \sigma(y; x)\bar{\phi}_t(y) + \phi_t(x)\gamma(y; y) + \phi_t(y)\gamma(x; y). \end{aligned} \quad (122)$$

We thus deduce that

$$\begin{aligned} i\partial_t\phi_t(x) &= \int h(x; y')\phi_t(y') dy' \\ &\quad + \int v(y - x)\phi_t(x)\gamma_t(y; y) dy + \int v(y - x)\phi_t(y)\gamma_t(x; y) dy \\ &\quad + \int v(x - y)\sigma_t(y, x)\bar{\phi}_t(y) dy + \int v(y - x)\phi_t(y)\phi_t(x)\bar{\phi}_t(y) dy \\ &= ((h + b[\gamma_t])\phi_t)(x) + k(\sigma_t^{\phi_t})\bar{\phi}_t(x) \end{aligned}$$

which is the dynamical Eq. (39) for ϕ_t .

For γ_t and σ_t , instead of ω_t^q we use

$$\omega_{C,t}^q(\mathbb{A}) := \omega_t^q(W_{\phi_t} \mathbb{A} W_{\phi_t}^*), \quad (123)$$

where, recall, $W_\phi = \exp(\psi^*(\phi) - \psi(\phi))$, the Weyl operators, which satisfy

$$W_\phi^* \psi(x) W_\phi = \psi(x) + \phi(x). \quad (124)$$

Note that the state $\omega_{C,t}^q$ is quasifree because ω_t^q is quasifree. By construction $\omega_{C,t}^q(\psi(x)) = 0$ and thus using (10) and the quasifreeness of $\omega_{C,t}^q$ one sees that $\omega_{C,t}^q$ vanishes on monomials of odd order in the fields. This provides substantial simplifications in the computations below.

In particular, the equations of the dynamics for γ_t and σ_t can be rewritten:

$$i \partial_t \gamma_t(x; y) = \omega_{C,t}^q([\psi^*(y) \psi(x), W_{\phi_t}^* \mathbb{H} W_{\phi_t}]) , \quad (125)$$

$$i \partial_t \sigma_t(x_1, y) = \omega_{C,t}^q([\psi(x_1) \psi(y), W_{\phi_t}^* \mathbb{H} W_{\phi_t}]) . \quad (126)$$

We compute $W_{\phi_t}^* \mathbb{H} W_{\phi_t}$ modulo terms of odd degree and of degree 0 in the creation and annihilation operators:

$$\begin{aligned} W_{\phi_t}^* \mathbb{H} W_{\phi_t} &\equiv \int \psi^*(z) (h + b_v[|\phi\rangle\langle\phi|])(z; z') \psi(z') \, dz dz' \\ &\quad + \frac{1}{2} \int v(z - z') \phi_t(z) \phi_t(z') \psi^*(z) \psi^*(z') \, dz dz' + adj. \\ &\quad + \frac{1}{2} \int v(z - z') \psi^*(z) \psi^*(z') \psi(z') \psi(z) \, dz dz' . \end{aligned} \quad (127)$$

Because $\omega_{C,t}^q$ vanishes on monomials of odd order in the fields and using the commutator, the knowledge of $W_{\phi_t}^* \mathbb{H} W_{\phi_t}$ modulo terms of odd degree and of degree 0 in the creation and annihilation operators is sufficient to compute the time derivative (125) of γ_t . Thus, using the CCR we get

$$\begin{aligned} i \partial_t \gamma_t(x; y) &= \int \omega_{C,t}^q \left((h + b_v[|\phi_t\rangle\langle\phi_t|])(x; z) \psi^*(y) \psi(z) \right. \\ &\quad - (h + B_v[|\phi_t\rangle\langle\phi_t|])(z; y) \psi^*(z) \psi(x) \\ &\quad + v(z - x) \phi_t(z) \phi_t(x) \psi^*(y) \psi^*(z) - v(z - y) \overline{\phi_t(z) \phi_t(y)} \psi(z) \psi(x) \\ &\quad \left. + v(z - x) \psi^*(y) \psi^*(z) \psi(x) \psi(z) - v(z - y) \psi^*(z) \psi^*(y) \psi(z) \psi(x) \right) dz . \end{aligned} \quad (128)$$

From the quasifreeness of $\omega_{C,t}^q$ follows:

$$\begin{aligned} i \partial_t \gamma_t(x; y) &= [h + b_v[|\phi_t\rangle\langle\phi_t| + \gamma_t], \gamma_t](x; y) \\ &\quad + \int (v(z - x) \phi_t(z) \phi_t(x) \overline{\sigma_t(y, z)} - v(z - y) \overline{\phi_t(z) \phi_t(y)} \sigma_t(z, x) \\ &\quad + v(z - x) \sigma_t(x, z) \overline{\sigma_t(y, z)} - v(z - y) \sigma_t(x, z) \overline{\sigma_t(y, z)}) \, dz . \end{aligned} \quad (129)$$

which is the dynamical Eq. (40) for γ_t .

Using the same arguments as for γ_t , we get

$$\begin{aligned}
 i\partial_t\sigma_t(x; y) &= \omega_{C,t}^q \left(v(x-y)\phi_t(x)\phi_t(y) + v(x-y)\psi(x)\psi(y) \right. \\
 &\quad + \int \left((h + b_v[|\phi_t\rangle\langle\phi_t|])(x; z)\psi(y) + (h + b_v[|\phi_t\rangle\langle\phi_t|])(y; z)\psi(x) \right) \psi(z) \\
 &\quad + v(x-z)\psi^*(z)\psi(y)\phi_t(x)\phi_t(z) + v(y-z)\psi^*(z)\psi(x)\phi_t(y)\phi_t(z) \\
 &\quad \left. + v(x-z)\psi^*(z)\psi(y)\psi(x)\psi(z) + v(y-z)\psi^*(z)\psi(x)\psi(y)\psi(z) \right) dz. \tag{130}
 \end{aligned}$$

From the quasifreeness of $\omega_{C,t}^q$ follows:

$$\begin{aligned}
 i\partial_t\sigma_t(x; y) &= v(x-y)\phi_t(x)\phi_t(y) + v(x-y)\sigma_t(x, y) \\
 &\quad + \int \left((h + b_v[|\phi_t\rangle\langle\phi_t|])(x; z)\sigma_t(y, z) + (h + b_v[|\phi_t\rangle\langle\phi_t|])(y; z)\sigma_t(x, z) \right. \\
 &\quad + v(x-z)\gamma_t(y; z)\phi_t(x)\phi_t(z) + v(y-z)\gamma_t(x; z)\phi_t(y)\phi_t(z) \\
 &\quad + v(x-z)(\gamma_t(x; z)\sigma_t(z, y) + \gamma_t(y; z)\sigma_t(z, x) + \gamma_t(z; z)\sigma_t(x, y)) \\
 &\quad \left. + v(y-z)(\gamma_t(x; z)\sigma_t(z, y) + \gamma_t(y; z)\sigma_t(z, x) + \gamma_t(z; z)\sigma_t(x, y)) \right) dz, \tag{131}
 \end{aligned}$$

which is the dynamical Eq. (41) for σ_t . $\square$

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A. Self-adjointness of the Hamiltonian $\mathbb{H}$

We use that the pair potential v is infinitesimally Δ -bounded, i.e., for any $\varepsilon \in (0, 1]$,

$$v \leq -\varepsilon \Delta + C\varepsilon^{-1} \quad (132)$$

(we write C for constants which depend on v , d and change along the estimates) to obtain after taking $\varepsilon = 1/(3(n-1))$,

$$v(x-y) \leq \frac{1}{6(n-1)}(-\Delta_x - \Delta_y) + C(n-1). \quad (133)$$

Then, summing the $n(n-1)/2$ terms of this form on each n -particles subspace of the Fock space, we obtain that

$$\mathbb{V} := \frac{1}{2} \int dx dy v(x-y) \psi^*(x) \psi^*(y) \psi(x) \psi(y) \leq \frac{2}{3} \mathbb{T} + C\mathbb{N}^3. \quad (134)$$

for some $C > 0$, with $\mathbb{T}$ defined in (86). One can then use the KLMN theorem and the Nelson theorem (see [40, 44]) to prove the self-adjointness of $\mathbb{H}$. (Details can be adapted from, e.g., [1, Section 3].)

B. Definition of quasifree states

For brevity, we write $\psi_j^\sharp := \psi^\sharp(x_j)$. We recall that the truncated expectations are defined via

$$\omega(\psi_1^\sharp \cdots \psi_n^\sharp) = \sum_{P_n} \prod_{J \in P_n} \omega^T\left(\prod_{j \in J} \psi_j^\sharp\right), \quad (135)$$

where P_n are partitions of the ordered set $\{1, \dots, n\}$ into ordered subsets.

We have $\omega^T(\psi) = \omega(\psi)$ and

$$\omega^T(\psi_1^\sharp \psi_2^\sharp) = \omega(\psi_1^\sharp \psi_2^\sharp) - \omega(\psi_1^\sharp) \omega(\psi_2^\sharp). \quad (136)$$

For quasifree states, the correlation functions $\omega(\psi_1^\sharp \cdots \psi_n^\sharp)$, with $n > 2$ can be expressed through $\omega(\psi^\sharp(x))$ and $\omega(\psi^\sharp(x) \psi^\sharp(y))$ according to the Wick formula. For

example,

$$\begin{aligned} \omega(\psi_1^\# \psi_2^\# \psi_3^\#) &= \omega(\psi_1^\#) \omega(\psi_2^\# \psi_3^\#) \\ &\quad + \omega(\psi_2^\#) \omega(\psi_1^* \psi_3^\#) + \omega(\psi_3^\#) \omega(\psi_1^\# \psi_2^\#) - 2 \prod_{i=1}^3 \omega(\psi_i^\#) \end{aligned} \quad (137)$$

and

$$\begin{aligned} \omega(\psi_1^\# \psi_2^\# \psi_3^\# \psi_4^\#) &= \omega(\psi_1^\# \psi_2^\#) \omega(\psi_3^\# \psi_4^\#) + \omega(\psi_1^\# \psi_3^\#) \omega(\psi_2^\# \psi_4^\#) \\ &\quad + \omega(\psi_1^\# \psi_4^\#) \omega(\psi_2^\# \psi_3^\#) - 2 \prod_{i=1}^4 \omega(\psi_i^\#) \end{aligned} \quad (138)$$

(remember that ψ 's stand on the right of ψ^* 's.) Note that

$$\omega(\psi^*(x)) = \overline{\omega(\psi(x))}, \quad \omega(\psi_1^* \psi_2^*) = \overline{\omega(\psi_2 \psi_1)}$$

and

$$\omega(\psi_1 \psi_2^*) = \omega(\psi_2^* \psi_1) + \delta(x - y).$$

Thus, a quasifree state ω is completely determined by the functions $\omega^T(\psi(x))$, $\omega^T(\psi^*(x)\psi(y))$ and $\omega^T(\psi(x)\psi(y))$.

Remark B.1. It is instructive to rewrite correlation functions for a quasifree state ω in terms of the fluctuation fields $\chi(x)$, defined as

$$\chi(x) := \psi(x) - \omega[\psi(x)], \quad (139)$$

where the average field $\omega[\psi(x)] = \phi(x)$ is considered a multiplication operator on $\mathcal{F}$. Then, ω is a quasifree state iff $\omega(\chi_1^\# \cdots \chi_{2n-1}^\#) = 0$ and

$$\omega(\chi_1^\# \cdots \chi_{2n}^\#) = \sum_{\pi \in S_n} \prod_{i=1}^{2n-1} \omega(\chi_{\pi(i)}^\# \chi_{\pi(i+1)}^\#),$$

where the sum is taken over all the permutations π of the set of indices $\{1, \dots, 2n\}$ satisfying $\pi(1) < \dots < \pi(2n)$ and, for all,

C. Equivalence of the HBF equations with the evolution generated by $\mathbb{H}_{hfb}(\omega_t^q)$

In this section, we prove Theorem 2.3.

Let a quasifree state ω_t^q satisfy (45) and let ϕ_t , γ_t and σ_t denote its truncated expectations. Below, we use the abbreviations $h(t) \equiv h(\gamma_t^{\phi_t})$ and $k(t) \equiv k(\sigma_t^{\phi_t})$, where,

recall, $\gamma^\phi := \gamma + |\phi\rangle\langle\phi|$ and $\sigma^\phi := \sigma + |\phi\rangle\langle\phi|$, and $h(\gamma)$ and $k(\sigma)$ are defined in (42) and (43). To find the equation for ϕ_t , we compute

$$\begin{aligned} i\partial_t\phi_t(x) &= \omega_t^q([\psi(x), \mathbb{H}_{hfb}(\omega_t^q)]) \\ &= \tilde{\omega}_t^q\left(\int h(t)(x; z)\psi(z)dz - b[|\phi_t\rangle\langle\phi_t|]\phi_t(x) + \int \psi^*(z)k(t)(x, z)dz\right) \\ &= h(t)\phi_t(x) - b[|\phi_t\rangle\langle\phi_t|]\phi_t(x) + k(t)\overline{\phi_t}(x). \end{aligned}$$

Hence ϕ_t satisfies (39).

For γ_t and σ_t we remark that, modulo terms of order one and constants $W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t}$ and $\mathbb{H}_{hfb}(\omega_t^q)$ coincide, hence

$$\begin{aligned} W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t} &\equiv \int h(t)(z; z')\psi^*(z)\psi(z')dzdz' \\ &\quad + \frac{1}{2} \int \psi^*(z_1)\psi^*(z_2)k(t)(z_1, z_2)dz_1dz_2 + adj.. \end{aligned} \quad (140)$$

Recall the definition (123) of $\omega_{C,t}^q(\mathbb{A})$. As in the proof of Theorem 2.2, the terms coming from the derivative of W_{ϕ_t} simplify:

$$i\partial_t\gamma_t(x; y) = \omega_{C,t}^q([\psi^*(y)\psi(x), W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t}]).$$

It is sufficient to consider $W_{\phi_t}^* \tilde{\mathbb{H}}(\phi_t, \gamma_t, \sigma_t) W_{\phi_t}$ modulo monomials of odd order in the fields:

$$\begin{aligned} i\partial_t\gamma_t(x; y) &= \omega_{C,t}^q\left(\int h(t)(x; z)\psi^*(x)\psi(z)dz - \int h(t)(z; y)\psi^*(z)\psi(y)dz\right. \\ &\quad \left.+ \int \psi^*(z)\psi^*(y)k(t)(z, x)dz - \int \overline{k(t)(z, y)}\psi(z)\psi(x)dz\right) \\ &= \int h(t)(x; z)\gamma_t(z; x)dz - \int \gamma_t(x; z)h_v(t)(z; y)dz \\ &\quad + \int \overline{\sigma_t(y, z)}k(t)(z, x)dz - \int \overline{k(t)(z, y)}\sigma_t(x, z)dz. \end{aligned}$$

Similarly

$$i\partial_t\sigma_t(x; y) = \omega_{C,t}^q([\psi(x)\psi(y), W_{\phi_t}^* \mathbb{H}_{hfb}(\omega_t^q) W_{\phi_t}]) \quad (141)$$

and

$$\begin{aligned} i\partial_t\gamma_t(x; y) &= \int h(t)(x; z)\sigma_t(x, z)dz + \int h(t)(y; z)\sigma_t(y, z)dz \\ &\quad + \int \gamma_t(y, z)k(t)(z, x)dz + \int \gamma_t(x, z)k(t)(z, y)dz + k(t)(x, y) \end{aligned} \quad (142)$$

Thus, γ_t and σ_t satisfy (40) and (41).

We have shown that, if a quasifree state ω_t^q satisfies (45), then its truncated expectations, ϕ_t , γ_t and σ_t , satisfy (39), (40) and (41). Proceeding in the opposite direction, one shows that, if truncated expectations, ϕ_t , γ_t and σ_t , satisfy (39), (40) and (41), then the corresponding quasifree state ω_t^q satisfies (45). $\square$

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