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ABSTRACT

We consider a gas of N bosons with interactions in the mean-field scaling regime. We review the proof of an asymptotic expansion of its low-energy spectrum, eigenstates, and dynamics, which provides corrections to Bogoliubov theory to all orders in $1/N$. This is based on joint works with Petrat, Pickl, Seiringer, and Soffer. In addition, we derive a full asymptotic expansion of the ground state one-body reduced density matrix.

I. INTRODUCTION AND MAIN RESULTS

A. Introduction

Since the first experimental realization of Bose–Einstein condensation (BEC) in 1995, the experimental, theoretical, and mathematical investigation of systems of interacting bosons at low temperatures has become a very active field of research. In a typical experiment, the bosons are initially caught in an external trap. This situation is mathematically described by the N-body Hamiltonian

$$H_N^{\text{trap}} = \sum_{j=1}^{N} \left(-\Delta_j + V^{\text{trap}}(x_j)\right) + \sum_{1\le i<j\le N} v_N(x_i - x_j) \tag{1.1}$$

for some confining potential V^{trap} and for some two-body interaction v_N, acting on the Hilbert space of square integrable, permutation symmetric functions on $\mathbb{R}^{dN}$,

$$\mathfrak{H}_{\text{sym}}^N := \bigotimes_{\text{sym}}^{N} \mathfrak{H}, \qquad \mathfrak{H} := L^2(\mathbb{R}^d).$$

The Bose gas is then cooled down to a low-energy eigenstate of H_N^{trap} or to a superposition of such states. For simplicity, let us assume that the gas is prepared in the ground state Ψ_N^{trap} of H_N^{trap}, i.e.,

$$\mathscr{E}_N^{\text{trap}} = \inf\sigma(H_N^{\text{trap}}), \qquad H_N^{\text{trap}}\Psi_N^{\text{trap}} = \mathscr{E}_N^{\text{trap}}\Psi_N^{\text{trap}}. \tag{1.2}$$

Subsequently, the trap is switched off and the Bose gas propagates freely. Mathematically, this is described by the N-body Schrödinger equation with initial datum Ψ_N^{trap},

$$\mathrm{i}\partial_t\Psi_N(t) = H_N\Psi_N(t), \qquad \Psi_N(0) = \Psi_N^{\text{trap}}, \tag{1.3}$$

with the N-body Hamiltonian

$$H_N = \sum_{j=1}^{N} (-\Delta_j) + \sum_{1\le i<j\le N} v_N(x_i - x_j). \tag{1.4}$$

Given that the number of particles in such a gas is usually large, an exact (analytical or numerical) analysis of the system in the presence of interactions is, in general, impossible; an exception is the explicitly solvable Lieb–Liniger model, which describes a one-dimensional gas with delta interactions. Over the last two decades, there have been many works in the mathematical physics community devoted to a rigorous derivation of suitable approximations of the statical and dynamical properties of the gas for large N. These questions have been studied for different classes of interactions v_N, in particular, for the so-called mean-field (or Hartree) regime,

$$v_N = \lambda_N v, \qquad \lambda_N := \frac{1}{N-1}, \tag{1.5}$$

describing the situation of weak and long-range interactions.

In this note, we consider interactions of the form (1.5). We present an asymptotic expansion of the low-energy spectrum and eigenstates of H_N^{trap} and of the dynamics (1.3), which makes the model fully computationally accessible to any order in $1/N$. This review is based on Ref. 1 (in collaboration with Petrat and Seiringer) and Ref. 2 (in collaboration with Petrat, Pickl, and Soffer).

B. Model and main results

We consider a system of N interacting bosons in $\mathbb{R}^d$, $d \ge 1$, which are described by the N-body Hamiltonian (1.1) with interactions (1.5). We impose the following assumptions on the interaction v_N and the external potential V^{trap}:

Assumption 1. Define v_N as in (1.5).

(a) *Let $v : \mathbb{R}^d \to \mathbb{R}$ be bounded with $v(-x) = v(x)$ and $v \not\equiv 0$.*
(b) *Assume that v is of positive type, i.e., that it has a non-negative Fourier transform.*

Assumption 2. Let $V^{\mathrm{trap}} : \mathbb{R}^d \to \mathbb{R}$ be measurable, locally bounded, and non-negative, and let $V^{\mathrm{trap}}(x)$ tend to infinity as $|x| \to \infty$.

Our first main result concerns the ground state Ψ_N^{trap} of H_N^{trap}: We construct a norm approximation of Ψ_N^{trap} and of its energy $\mathscr{E}_N^{\mathrm{trap}}$ to any order in $1/N$.

Theorem 1. *Let $a \in \mathbb{N}_0$, let Assumptions 1 and 2 be satisfied, and choose N sufficiently large. Then, there exists a constant $C(a)$ such that*

$$\left\| \Psi_N^{\mathrm{trap}} - \sum_{\ell=0}^{a} \lambda_N^{\frac{\ell}{2}} \psi_{N,\ell}^{\mathrm{trap}} \right\|_{\mathfrak{H}^N} \le C(a) \lambda_N^{\frac{a+1}{2}} \tag{1.6}$$

and

$$\left| \mathscr{E}_N^{\mathrm{trap}} - N e_{\mathrm{H}}^{\mathrm{trap}} - \sum_{\ell=0}^{a} \lambda_N^{\ell} E_\ell^{\mathrm{trap}} \right| \le C(a) \lambda_N^{a+1}. \tag{1.7}$$

The coefficients $\psi_{N,\ell}^{\mathrm{trap}} \in \mathfrak{H}_{\mathrm{sym}}^N$ of expansion (1.6) and the coefficients $e_{\mathrm{H}}^{\mathrm{trap}}$, $E_\ell^{\mathrm{trap}} \in \mathbb{R}$ of expansion (1.7) are given in (2.46), (2.4), and (2.47), respectively.

Our result extends to the low-energy excitation spectrum of H_N^{trap} and to a certain class of unbounded interaction potentials v, including the repulsive three-dimensional Coulomb potential (see Sec. II E). To leading order $(a = 0)$, the statements (1.6) and (1.7) have been proven (for bounded interactions) by Seiringer on the torus[3] and by Grech and Seiringer in the inhomogeneous setting.[4] For our class of unbounded interactions, the leading order approximation was obtained by Lewin, Nam, Serfaty, and Solovej.[5] The higher orders in (1.6) and (1.7) were, to the best of our knowledge, first rigorously derived in Ref. 1. Another approach was proposed by Pizzo in Refs. 6–8, who considers a Bose gas on a torus and constructs an expansion for the ground state, based on a multi-scale analysis in the number of excitations, around a product state using Feshbach maps. As a consequence of the norm approximation (1.6), one can derive an expansion of the ground state one-body reduced density matrix,

$$\gamma_N^{\mathrm{trap},(1)} := \mathrm{Tr}_{\mathfrak{H}^{N-1}} |\Psi_N^{\mathrm{trap}}\rangle\langle\Psi_N^{\mathrm{trap}}|, \tag{1.8}$$

in trace norm (see Sec. II D for a proof of this statement).

Corollary 1.1. Let $a \in \mathbb{N}_0$, and let Assumptions 1 and 2 be satisfied. Denote by $\gamma_N^{\mathrm{trap},(1)}$ the one-body reduced density matrix of Ψ_N^{trap}. Then, there exists a constant $C(a) > 0$ such that

$$\operatorname{Tr}\left|\gamma_N^{\mathrm{trap},(1)} - \sum_{\ell=0}^{a} \lambda_N^{\ell} \gamma_{1,\ell}^{\mathrm{trap}}\right| \le C(a)\lambda_N^{a+1} \tag{1.9}$$

for sufficiently large N, where the coefficients $\gamma_{1,\ell}^{\mathrm{trap}} \in \mathcal{L}(\mathfrak{H})$ are defined in (2.50).

Theorem 1 and Corollary 1.1 determine the ground state Ψ_N^{trap} of H_N^{trap} to arbitrary precision. Now, we remove the confining potential V^{trap} and take Ψ_N^{trap} as initial datum for the time evolution (1.3). Since an eigenstate of H_N^{trap} is not necessarily an eigenstate of H_N, this leads to some non-trivial dynamics, for which we provide an approximation in norm to any order in $1/N$ in our second main result.

Theorem 2. *Let $a \in \mathbb{N}_0$, $t \in \mathbb{R}$, let Assumption 1a hold, and denote by $\Psi_N(t)$ the solution of (1.3). Then, there exists a constant $C(a) > 0$ such that*

$$\left\|\Psi_N(t) - \sum_{\ell=0}^{a} \lambda_N^{\frac{\ell}{2}} \psi_{N,\ell}(t)\right\|_{\mathfrak{H}^N} \le \mathrm{e}^{C(a)t} \lambda_N^{\frac{a+1}{2}} \tag{1.10}$$

for sufficiently large N, where the coefficients $\psi_{N,\ell}(t)$ are defined in (3.19).

Note that for the dynamical result, we do not require the interaction potential to be of positive type. Finally, we derive from expansion (1.10) a trace norm approximation of the time-evolved one-body reduced density matrix

$$\gamma_N^{(1)}(t) := \operatorname{Tr}_{\mathfrak{H}^{N-1}} |\Psi_N(t)\rangle\langle\Psi_N(t)| \tag{1.11}$$

to arbitrary precision.

Corollary 1.2. Let $a \in \mathbb{N}_0$, $t \in \mathbb{R}$, and let Assumption 1a be satisfied. Then, there exists a constant $C(a)$ such that

$$\operatorname{Tr}\left|\gamma_N^{(1)}(t) - \sum_{\ell=0}^{a} \lambda_N^{\ell} \gamma_{1,\ell}(t)\right| \le \mathrm{e}^{C(a)t} \lambda_N^{a+1} \tag{1.12}$$

for sufficiently large N, where the coefficients $\gamma_{1,\ell}(t) \in \mathcal{L}(\mathfrak{H})$ are defined in (3.26).

Below, we will provide and explain the explicit formulas for the coefficients in Theorems 1 and 2 and in Corollaries 1.1 and 1.2. Note that $e_{\mathrm{H}}^{\mathrm{trap}}$, E_ℓ^{trap}, $\gamma_{1,\ell}^{\mathrm{trap}}$, and $\gamma_{1,\ell}(t)$ are completely independent of N. The N-body wave functions $\psi_{N,\ell}^{\mathrm{trap}}$ and $\psi_{N,\ell}(t)$ naturally depend on N; however, this N-dependence is trivial in a sense to be made precise below. In particular, the computational effort to obtain physical quantities, such as expectation values of bounded operators with respect to the (time-evolved) N-body state, does not scale with N.

Finally, let us remark that all constants $C(a)$ grow rapidly in a. Hence, all statements are to be read as *asymptotic* expansions: given any order a of the approximation, one can choose N sufficiently large such that the estimates are meaningful, but we cannot simultaneously send a to infinity.

To prove the above results, we first remove the particles in the condensate from the description and focus only on the excitations from the condensate. Mathematically, this is done by conjugating the N-body Hamiltonians with a unitary map that maps from the N-body Hilbert space into a truncated Fock space, whose elements describe the excitations. The resulting operator is then expanded in the parameter $\lambda_N^{1/2}$, which (formally) leads to a series of the form

$$\mathbb{H} = \mathbb{H}_0 + \sum_{j \ge 1} \lambda_N^{\frac{j}{2}} \mathbb{H}_j,$$

where the leading order term $\mathbb{H}_0$ is the well-known Bogoliubov Hamiltonian. Formally, our results can be obtained by perturbation theory around $\mathbb{H}_0$ to any order; however, the rigorous proofs are much more involved, mainly since all operators are unbounded and non-commutative.

This Review is organized as follows: In Sec. II, we explain the results from Ref. 1 concerning the low-energy spectrum and eigenstates and give a proof of Corollary 1.1. Section III contains the results for the dynamics obtained in Ref. 2.

We use the following notations:

- The notation $A \lesssim B$ indicates that there exists a constant $C > 0$ such that $A \le CB$.
- For $k \ge 1$ and $x_j \in \mathbb{R}^d$, we abbreviate $x^{(k)} := (x_1, \ldots, x_k)$ and $\mathrm{d}x^{(k)} := \mathrm{d}x_1 \cdots \mathrm{d}x_k$.
- We use the notation $a^{\sharp_1} := a^\dagger$ and $a^{\sharp_{-1}} := a$.
- Multi-indices are denoted as $\boldsymbol{j} = (j_1, \ldots, j_n)$ with $|\boldsymbol{j}| := j_1 + \cdots + j_n$.

II. LOW-ENERGY SPECTRUM AND EIGENSTATES

In this section, we consider the Hamiltonian H_N^{trap} from (1.1) and explain the asymptotic expansion of its ground state Ψ_N^{trap}, the ground state energy $\mathscr{E}_N^{\mathrm{trap}}$, and the corresponding reduced density matrix $\gamma_N^{\mathrm{trap},(1)}$. To keep the notation simple, we drop the superscript$^{\mathrm{trap}}$.

A. Framework

1. Condensate

It is well known (see, e.g., Refs. 3–5 and 9) that the N-body ground state Ψ_N exhibits (complete asymptotic) BEC in the minimizer $\varphi \in \mathfrak{H}$ of the Hartree energy functional $\mathcal{E}_{\mathrm{H}}$,

$$\mathcal{E}_{\mathrm{H}}[\phi] := \int_{\mathbb{R}^d} \left(|\nabla\phi(x)|^2 + V(x)|\phi(x)|^2\right)\mathrm{d}x + \frac{1}{2}\int_{\mathbb{R}^{2d}} v(x-y)|\phi(x)|^2|\phi(y)|^2\mathrm{d}x\mathrm{d}y. \tag{2.1}$$

For potentials v and V satisfying Assumptions 1 and 2, the minimizer φ of $\mathcal{E}_{\mathrm{H}}$ is unique, strictly positive, and solves the stationary Hartree equation

$$h\varphi := \left(-\Delta + V + v * \varphi^2 - \mu_{\mathrm{H}}\right)\varphi = 0 \tag{2.2}$$

with the Lagrange parameter $\mu_{\mathrm{H}} := \langle\varphi, (-\Delta + V + v * \varphi^2)\varphi\rangle \in \mathbb{R}$. We denote by p^φ and q^φ the projector onto φ and its orthogonal complement, i.e.,

$$p^\varphi := |\varphi\rangle\langle\varphi|, \quad q^\varphi := \mathbb{1} - p^\varphi. \tag{2.3}$$

The minimum of $\mathcal{E}_{\mathrm{H}}$ is given as

$$e_{\mathrm{H}} := \mathcal{E}_{\mathrm{H}}[\varphi] = \left\langle\varphi, \left(-\Delta + V + \frac{1}{2}v * \varphi^2\right)\varphi\right\rangle. \tag{2.4}$$

Heuristically, (complete asymptotic) BEC in the state φ means that $N - o(N)$ particles occupy the condensate state φ. Mathematically, this is reflected by the fact that the N-body wave function is determined by the one-body state φ in the sense of reduced densities, i.e.,

$$\lim_{N\to\infty} \mathrm{Tr}\left|\gamma_N^{(1)} - |\varphi\rangle\langle\varphi|\right| = 0. \tag{2.5}$$

The condensate determines the leading order of the ground state energy, namely,

$$\mathscr{E}_N = Ne_{\mathrm{H}} + \mathcal{O}(1). \tag{2.6}$$

2. Excitations

The errors in (2.5) and (2.6) are caused by $\mathcal{O}(1)$ particles that are excited from the condensate due to the inter-particle interactions. To describe these excitations, we decompose Ψ_N as

$$\Psi_N = \sum_{k=0}^{N} \varphi^{\otimes(N-k)} \bigotimes_s \chi^{(k)}, \qquad \chi^{(k)} \in \bigotimes_{\mathrm{sym}}^{k} \mathfrak{H}_{\perp\varphi}, \tag{2.7}$$

with $\otimes_s$ being the symmetric tensor product and where $\mathfrak{H}_{\perp\varphi} := \{\phi \in \mathfrak{H} : \langle\phi, \varphi\rangle_{\mathfrak{H}} = 0\}$ denotes the orthogonal complement of φ in $\mathfrak{H}$.[5] The excitations

$$\boldsymbol{\chi}_{\leq N} := \left(\chi^{(k)}\right)_{k=0}^{N} \tag{2.8}$$

form a vector in the truncated (excitation) Fock space over $\mathfrak{H}_{\perp\varphi}$,

$$\mathcal{F}_{\perp\varphi}^{\leq N} = \bigoplus_{k=0}^{N} \bigotimes_{\mathrm{sym}}^{k} \mathfrak{H}_{\perp\varphi} \subset \mathcal{F}_{\perp\varphi} = \bigoplus_{k\geq 0}^{\infty} \bigoplus_{\mathrm{sym}} \mathfrak{H}_{\perp\varphi} \subset \mathcal{F} = \bigoplus_{k\geq 0} \bigotimes_{\mathrm{sym}}^{k} \mathfrak{H}, \tag{2.9}$$

which is a subspace of the Fock space $\mathcal{F}$ over $\mathfrak{H}$. The creation/annihilation operators $a^\dagger/a$ on $\mathcal{F}$ are defined in the usual way, and we denote the second quantization in $\mathcal{F}$ of an operator T on $\mathfrak{H}$ by $\mathrm{d}\Gamma(T)$. The number operator on $\mathcal{F}_{\perp\varphi}$ is given by

$$\mathcal{N}_{\perp\varphi} := \mathrm{d}\Gamma(q^{\varphi}). \tag{2.10}$$

The relation between Ψ_N and the corresponding excitation vector $\boldsymbol{\chi}_{\leq N}$ is given by the unitary map

$$\mathfrak{U}_{N,\varphi} : \mathfrak{H}^N \to \mathcal{F}_{\perp\varphi}^{\leq N}, \quad \Psi \mapsto \mathfrak{U}_{N,\varphi}\Psi = \boldsymbol{\chi}_{\leq N}, \tag{2.11}$$

whose action is explicitly known [see Ref. 5 (Proposition 4.2)]. Conjugating H_N with $\mathfrak{U}_{N,\varphi}$ yields the operator

$$\mathbb{H}_{\leq N} := \mathfrak{U}_{N,\varphi}(H_N - Ne_{\mathrm{H}})\mathfrak{U}_{N,\varphi}^{*} \tag{2.12}$$

on $\mathcal{F}_{\perp\varphi}^{\leq N}$, whose ground state is given by $\boldsymbol{\chi}_{\leq N}$. Hence, the ground state energy of $\mathbb{H}_{\leq N}$,

$$E_{\leq N} := \inf\sigma(\mathbb{H}_{\leq N}) = \langle \boldsymbol{\chi}_{\leq N}, \mathbb{H}_{\leq N}\boldsymbol{\chi}_{\leq N}\rangle_{\mathcal{F}_{\perp\varphi}^{\leq N}} = \mathscr{E}_N - Ne_{\mathrm{H}}, \tag{2.13}$$

is precisely the $\mathcal{O}(1)$-term in (2.6).

3. Excitation Hamiltonian

Making use of the explicit form of $\mathfrak{U}_{N,\varphi}$ [Ref. 5 (Proposition 4.2)], we can express $\mathbb{H}_{\leq N}$ as

$$\begin{aligned}\mathbb{H}_{\leq N} = \mathbb{K}_0 + \left(\frac{N-\mathcal{N}_{\perp\varphi}}{N-1}\right)\mathbb{K}_1 + \left(\mathbb{K}_2\frac{\sqrt{(N-\mathcal{N}_{\perp\varphi})(N-\mathcal{N}_{\perp\varphi}-1)}}{N-1} + \frac{\sqrt{(N-\mathcal{N}_{\perp\varphi})(N-\mathcal{N}_{\perp\varphi}-1)}}{N-1}\mathbb{K}_2^{*}\right)\\ +\left(\mathbb{K}_3\frac{\sqrt{N-\mathcal{N}_{\perp\varphi}}}{N-1} + \frac{\sqrt{N-\mathcal{N}_{\perp\varphi}}}{N-1}\mathbb{K}_3^{*}\right) + \frac{1}{N-1}\mathbb{K}_4\end{aligned} \tag{2.14}$$

as an operator on $\mathcal{F}_{\perp\varphi}^{\leq N}$, where we used the shorthand notation

$$\mathbb{K}_0 := \mathrm{d}\Gamma(h), \qquad \mathbb{K}_1 := \mathrm{d}\Gamma(K_1), \qquad \mathbb{K}_4 := \mathrm{d}\Gamma(K_4), \tag{2.15a}$$

$$\mathbb{K}_2 := \frac{1}{2}\int \mathrm{d}x_1\mathrm{d}x_2\, K_2(x_1,x_2)a_{x_1}^{\dagger}a_{x_2}^{\dagger}, \tag{2.15b}$$

$$\mathbb{K}_3 := \int \mathrm{d}x^{(3)}\, K_3(x_1,x_2;x_3)a_{x_1}^{\dagger}a_{x_2}^{\dagger}a_{x_3} \tag{2.15c}$$

for h as in (2.2) and where

$$K_1 : \mathfrak{H}_{\perp\varphi} \to \mathfrak{H}_{\perp\varphi}, \qquad K_1 := q^{\varphi}Kq^{\varphi}, \tag{2.16a}$$

$$K_2 \in \mathfrak{H}_{\perp\varphi} \otimes \mathfrak{H}_{\perp\varphi}, \qquad K_2(x_1,x_2) := (q_1^{\varphi}q_2^{\varphi}K)(x_1,x_2), \tag{2.16b}$$

$$K_3 : \mathfrak{H}_{\perp\varphi} \to \mathfrak{H}_{\perp\varphi} \otimes \mathfrak{H}_{\perp\varphi}, \quad (K_3\psi)(x_1,x_2) := q_1^{\varphi}q_2^{\varphi}W(x_1,x_2)\varphi(x_1)(q_2^{\varphi}\psi)(x_2), \tag{2.16c}$$

$$K_4 : \mathfrak{H}_{\perp\varphi} \otimes \mathfrak{H}_{\perp\varphi} \to \mathfrak{H}_{\perp\varphi} \otimes \mathfrak{H}_{\perp\varphi}, \quad (K_4\psi)(x_1,x_2) := q_1^{\varphi}q_2^{\varphi}W(x_1,x_2)(q_1^{\varphi}q_2^{\varphi}\psi)(x_1,x_2). \tag{2.16d}$$

Here, $K(x_1,x_2)$ is defined as

$$K(x_1;x_2) := v(x_1-x_2)\varphi(x_1)\varphi(x_2), \tag{2.17}$$

K is the operator with kernel $K(x_1,x_2)$, and W is the multiplication operator defined by

$$W(x_1,x_2) := v(x_1-x_2) - (v*\varphi^2)(x_1) - (v*\varphi^2)(x_2) + \langle\varphi, v*\varphi^2\varphi\rangle. \tag{2.18}$$

By construction, $\mathbb{H}_{\leq N}$ is explicitly N-dependent. To extract its contributions to each order in λ_N, we first extend $\mathbb{H}_{\leq N}$ trivially to an operator on $\mathcal{F}_{\perp\varphi}$,

$$\mathbb{H} := \mathbb{H}_{\leq N} \oplus c, \tag{2.19}$$

where the direct sum is with respect to the decomposition $\mathcal{F} = \mathcal{F}^{\le N} \oplus \mathcal{F}^{<N}$. The constant c in (2.19) will later be chosen conveniently (see Sec. II C). Similarly, we extend $\chi_{\le N}$ to a vector $\chi \in \mathcal{F}_{\perp\varphi}$ as

$$\chi := \chi_{\le N} \oplus 0 \tag{2.20}$$

and denote the corresponding projectors on $\mathcal{F}_{\perp\varphi}$ by

$$\mathbb{P} := |\chi\rangle\langle\chi|, \qquad \mathbb{Q} := \mathbb{1} - \mathbb{P}. \tag{2.21}$$

A (formal) expansion of $\mathbb{H}$ in powers of $\lambda_N^{1/2}$ yields

$$\mathbb{H} = \mathbb{H}_0 + \sum_{j\ge 1} \lambda_N^{\frac{j}{2}} \mathbb{H}_j, \tag{2.22}$$

where

$$\mathbb{H}_0 := \mathbb{K}_0 + \mathbb{K}_1 + \mathbb{K}_2 + \mathbb{K}_2^*, \tag{2.23a}$$

$$\mathbb{H}_1 := \mathbb{K}_3 + \mathbb{K}_3^*, \tag{2.23b}$$

$$\mathbb{H}_2 := -(\mathcal{N}_{\perp\varphi} - 1)\mathbb{K}_1 - \left(\mathbb{K}_2\left(\mathcal{N}_{\perp\varphi} - \frac{1}{2}\right) + \text{h.c.}\right) + \mathbb{K}_4, \tag{2.23c}$$

$$\mathbb{H}_{2j-1} := c_{j-1}\left(\mathbb{K}_3(\mathcal{N}_{\perp\varphi} - 1)^{j-1} + \text{h.c.}\right), \tag{2.23d}$$

$$\mathbb{H}_{2j} := \sum_{\nu=0}^{j} d_{j,\nu}\left(\mathbb{K}_2(\mathcal{N}_{\perp\varphi} - 1)^{\nu} + \text{h.c.}\right) \tag{2.23e}$$

for $j \ge 2$, with $\mathbb{K}_j$ as in (2.15). The coefficients c_j and $d_{j,\nu}$ are given as

$$c_0^{(\ell)} := 1, \quad c_j^{(\ell)} := \frac{\left(\ell - \frac{1}{2}\right)\left(\ell + \frac{1}{2}\right)\left(\ell + \frac{3}{2}\right)\cdots\left(\ell + j - \frac{3}{2}\right)}{j!}, \quad c_j := c_j^{(0)} \quad (j \ge 1), \tag{2.24a}$$

$$d_{j,\nu} := \sum_{\ell=0}^{\nu} c_\ell^{(0)} c_{\nu-\ell}^{(0)} c_{j-\nu}^{(\ell)} \qquad (j \ge \nu \ge 0). \tag{2.24b}$$

4. Bogoliubov approximation

The leading order term $\mathbb{H}_0$ in (2.22) is the well-known Bogoliubov Hamiltonian. We denote the unique ground state of $\mathbb{H}_0$ and the ground state energy by

$$E_0 := \inf \sigma(\mathbb{H}_0), \qquad \mathbb{H}_0 \chi_0 = E_0 \chi_0, \tag{2.25}$$

and the corresponding projectors are defined as

$$\mathbb{P}_0 := |\chi_0\rangle\langle\chi_0|, \qquad \mathbb{Q}_0 := \mathbb{1} - \mathbb{P}_0. \tag{2.26}$$

It is well known[3–5] that the ground state $\chi_{\le N}$ of $\mathbb{H}_{\le N}$ and the ground state energy $E_{\le N}$ converge to χ_0 and E_0, respectively, i.e.,

$$\lim_{N\to\infty} E_{\le N} = E_0, \qquad \lim_{N\to\infty} \|\chi_{\le N} - \chi_0\|_{\mathcal{F}_{\perp\varphi}^{\le N}} = 0. \tag{2.27}$$

Consequently, E_0 gives the next-to-leading order term in (1.7); analogously, the leading order contribution in (1.6) is given by $\psi_{N,0} = \mathfrak{U}_{N,\varphi}^* \chi_0|_{\mathcal{F}_{\perp\varphi}^{\le N}}$.

The Bogoliubov Hamiltonian $\mathbb{H}_0$ is a very useful approximation of $\mathbb{H}$ because it is much simpler than the full problem: it is quadratic in the number of creation/annihilation operators and can be diagonalized by Bogoliubov transformations.

Let us briefly recall the concept of Bogoliubov transformations. For $F = f \oplus Jg \in \mathfrak{H} \oplus \mathfrak{H}$, where $J : \mathfrak{H} \to \mathfrak{H}$ denotes complex conjugation, one defines the generalized creation and annihilation operators $A(F)$ and $A^\dagger(F)$ as

$$A(F) = a(f) + a^\dagger(g), \quad A^\dagger(F) = A(\mathcal{J}F) = a^\dagger(f) + a(g) \tag{2.28}$$

for $\mathcal{J} = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix}$. An operator $\mathcal{V}$ on $\mathfrak{H} \oplus \mathfrak{H}$ such that $F \mapsto A(\mathcal{V}F)$ has the same properties as $F \mapsto A(F)$, i.e., $A^\dagger(\mathcal{V}F) = A(\mathcal{V}\mathcal{J}F)$ and $[A(\mathcal{V}F_1), A^\dagger(\mathcal{V}F_2)] = [A(F_1), A^\dagger(F_2)]$, is called a *(bosonic) Bogoliubov map* and can be written in block form as

$$\mathcal{V} := \begin{pmatrix} U & \overline{V} \\ V & \overline{U} \end{pmatrix}, \quad U, V : \mathfrak{H}_{\perp\varphi} \to \mathfrak{H}_{\perp\varphi}. \tag{2.29}$$

If V is Hilbert–Schmidt, the Bogoliubov map $\mathcal{V}$ can be unitarily implemented on $\mathcal{F}$, i.e., there exists a unitary transformation $\mathbb{U}_{\mathcal{V}} : \mathcal{F} \to \mathcal{F}$ (called a *Bogoliubov transformation*) such that $\mathbb{U}_{\mathcal{V}} A(F) \mathbb{U}_{\mathcal{V}}^* = A(\mathcal{V}F)$ for all $F \in \mathfrak{H} \oplus \mathfrak{H}$. This implies the transformation rule

$$\mathbb{U}_{\mathcal{V}}\, a(f)\, \mathbb{U}_{\mathcal{V}}^* = a(Uf) + a^\dagger(\overline{Vf}), \qquad \mathbb{U}_{\mathcal{V}}\, a^\dagger(f)\, \mathbb{U}_{\mathcal{V}}^* = a^\dagger(Uf) + a(\overline{Vf}). \tag{2.30}$$

A normalized state $\boldsymbol{\phi} \in \mathcal{F}_{\perp\varphi}$ that can be written as

$$\boldsymbol{\phi} = \mathbb{U}_{\mathcal{V}} |\Omega\rangle \tag{2.31}$$

for some Bogoliubov map $\mathcal{V}$ is called a *quasi-free state*. Quasi-free states have a finite expectation value of the number operator and satisfy Wick's rule, i.e.,

$$\left\langle \boldsymbol{\phi}, a^\sharp(f_1) \cdots a^\sharp(f_{2n-1}) \boldsymbol{\phi} \right\rangle_{\mathcal{F}_{\perp\varphi}} = 0, \tag{2.32a}$$

$$\left\langle \boldsymbol{\phi}, a^\sharp(f_1) \cdots a^\sharp(f_{2n}) \boldsymbol{\phi} \right\rangle_{\mathcal{F}_{\perp\varphi}} = \sum_{\sigma \in P_{2n}} \prod_{j=1}^{n} \left\langle \boldsymbol{\phi}, a^\sharp(f_{\sigma(2j-1)}) a^\sharp(f_{\sigma(2j)}) \boldsymbol{\phi} \right\rangle_{\mathcal{F}_{\perp\varphi}} \tag{2.32b}$$

for $a^\sharp \in \{a^\dagger, a\}$, $n \in \mathbb{N}$, and $f_1, \ldots, f_{2n} \in \mathfrak{H}_{\perp\varphi}$. Here, P_{2n} denotes the set of pairings

$$P_{2n} := \{\sigma \in \mathfrak{S}_{2n} : \sigma(2a-1) < \min\{\sigma(2a), \sigma(2a+1)\}\ \forall a \in \{1, 2, \ldots, 2n\}\}, \tag{2.33}$$

for $\mathfrak{S}_{2n}$ the symmetric group on the set $\{1, 2, \ldots, 2n\}$. In particular, the ground state $\boldsymbol{\chi}_0$ of $\mathbb{H}_0$ is a quasi-free state,

$$\boldsymbol{\chi}_0 = \mathbb{U}_{\mathcal{V}_0}^* |\Omega\rangle, \tag{2.34}$$

where $\mathbb{U}_{\mathcal{V}_0}$ is the Bogoliubov transformation that diagonalizes $\mathbb{H}_0$.

B. Expansion of the ground state

To prove Theorem 1, we show that the projector $\mathbb{P}$ from (2.21) admits a series expansion in powers of $\lambda_N^{1/2}$ in the following sense:

Proposition 2.1. Let Assumptions 1 and 2 hold, let $\mathbb{A} \in \mathcal{L}(\mathcal{F}_{\perp\varphi})$ be a bounded operator on $\mathcal{F}_{\perp\varphi}$, and let $a \in \mathbb{N}_0$. Then, there exists some constant $C(a)$ such that

$$\left| \mathrm{Tr}\, \mathbb{A}\mathbb{P} - \sum_{\ell=0}^{a} \lambda_N^{\frac{\ell}{2}} \mathrm{Tr}\, \mathbb{A}\mathbb{P}_\ell \right| \le C(a) \lambda_N^{\frac{a+1}{2}} \|\mathbb{A}\|_{\mathrm{op}} \tag{2.35}$$

for sufficiently large N, where $\|\cdot\|_{\mathrm{op}}$ denotes the operator norm. The coefficients $\mathbb{P}_\ell$ are defined as

$$\mathbb{P}_\ell := \begin{cases} \mathbb{P}_0 & \text{if } \ell = 0, \\ -\sum\limits_{\nu=1}^{\ell} \sum\limits_{\substack{\boldsymbol{j} \in \mathbb{N}^\nu \\ |\boldsymbol{j}| = \ell}} \sum\limits_{\substack{\boldsymbol{k} \in \mathbb{N}_0^{\nu+1} \\ |\boldsymbol{k}| = \nu}} \mathbb{O}_{k_1} \mathbb{H}_{j_1} \mathbb{O}_{k_2} \mathbb{H}_{j_2} \cdots \mathbb{O}_{k_\nu} \mathbb{H}_{j_\nu} \mathbb{O}_{k_{\nu+1}} & \text{if } \ell \ge 1, \end{cases} \tag{2.36}$$

with $\mathbb{P}_0$ as in (2.26) and $\mathbb{H}_j$ as in (2.23) and where we abbreviated

$$\mathbb{O}_k := \begin{cases} -\mathbb{P}_0 & k = 0, \\ \dfrac{\mathbb{Q}_0}{(E_0 - \mathbb{H}_0)^k} & k > 0. \end{cases} \tag{2.37}$$

The growth of the constant $C(a)$ in the order a of the approximation can be estimated as

$$C(a) \le C(a+1)^{(a+6)^2},$$

which we expect to be far from optimal. By means of Bogoliubov transformations, the operators $\mathbb{P}_\ell$ can be brought into a more explicit form. For example, the first order correction $\mathbb{P}_1$ is given by

$$\mathbb{P}_1 = \mathbb{U}_{\mathcal{V}_0}^*\big(\mathbb{U}_{\mathcal{V}_0}\mathbb{O}_1\mathbb{U}_{\mathcal{V}_0}^*\big)\big(\mathbb{U}_{\mathcal{V}_0}\mathbb{H}_1\mathbb{U}_{\mathcal{V}_0}^*\big)|\Omega\rangle\langle\chi_0| + \text{h.c.}, \tag{2.38}$$

where $\mathbb{U}_{\mathcal{V}_0}$ is the Bogoliubov transformation diagonalizing $\mathbb{H}_0$ such that $\chi_0 = \mathbb{U}_{\mathcal{V}_0}^*|\Omega\rangle$. To simplify (2.38), one notes that $\mathbb{U}_{\mathcal{V}_0}\mathbb{H}_1\mathbb{U}_{\mathcal{V}_0}^*|\Omega\rangle$ is a superposition of one- and three-particle states and that $\mathbb{U}_{\mathcal{V}_0}\mathbb{O}_1^{(0)}\mathbb{U}_{\mathcal{V}_0}^*$ is particle-number preserving. Hence, $\mathbb{P}_1$ can be expressed as

$$\mathbb{P}_1 = \mathbb{U}_{\mathcal{V}_0}^*\bigg(\int \mathrm{d}x\,\Theta_1(x)a_x^\dagger|\Omega\rangle + \int \mathrm{d}x^{(3)}\Theta_3(x^{(3)})a_{x_1}^\dagger a_{x_2}^\dagger a_{x_3}^\dagger|\Omega\rangle\bigg)\langle\chi_0| + \text{h.c.}, \tag{2.39}$$

where the functions Θ_1 and Θ_3 can be retrieved by diagonalizing $\mathbb{H}_0$ and computing the Bogoliubov transformation of $\mathbb{H}_1$ under $\mathbb{U}_{\mathcal{V}_0}$.

From Proposition 2.1, we deduce three consequences.

1. Ground state wave function

As an immediate consequence of Proposition 2.1, we find that

$$\operatorname{Tr}\bigg|\mathbb{P} - \sum_{\ell=0}^{a}\lambda_N^{\frac{\ell}{2}}\mathbb{P}_\ell\bigg| \le C(a)\lambda_N^{\frac{a+1}{2}}. \tag{2.40}$$

Since $\mathbb{P} = |\chi\rangle\langle\chi|$ is a rank one projector, expansion (2.40) implies an expansion of the excitation wave function χ,

$$\bigg\|\chi - \sum_{\ell=0}^{a}\lambda_N^{\frac{\ell}{2}}\chi_\ell\bigg\|_{\mathcal{F}} \le C(a)\lambda_N^{\frac{a+1}{2}} \tag{2.41}$$

[see Ref. 1 (Appendix B) for a proof of this statement in a general Hilbert space setting]. The coefficients of the expansion are given by

$$\chi_\ell := \sum_{j=0}^{\ell}\alpha_j\widetilde{\chi}_{\ell-j} \qquad (\ell \ge 1), \tag{2.42}$$

where

$$\widetilde{\chi}_\ell := \sum_{\nu=1}^{\ell}\sum_{\substack{\boldsymbol{j}\in\mathbb{N}^\nu\\ |\boldsymbol{j}|=\ell}}\mathbb{P}_{j_1}\cdots\mathbb{P}_{j_\nu}\chi_0 \qquad (\ell \ge 1), \tag{2.43}$$

with $\mathbb{P}_\ell$ as in (2.36) and χ_0 as in (2.25), and for $n \ge 1$,

$$\alpha_0 := 1, \qquad \alpha_{2n-1} := 0, \qquad \alpha_{2n} := -\frac{1}{2}\sum_{\substack{\boldsymbol{j}\in\mathbb{N}_0^4\\ j_1,j_2<2n\\ |\boldsymbol{j}|=2n}}\alpha_{j_1}\alpha_{j_2}\langle\widetilde{\chi}_{j_3},\widetilde{\chi}_{j_4}\rangle. \tag{2.44}$$

For example,

$$\chi_1 = \frac{\mathbb{Q}_0}{E_0 - \mathbb{H}_0}\mathbb{H}_1\chi_0 = \mathbb{U}_{\mathcal{V}_0}^*\bigg(\int \mathrm{d}x\,\Theta_1(x)a_x^\dagger|\Omega\rangle + \int \mathrm{d}x^{(3)}\Theta_3(x^{(3)})a_{x_1}^\dagger a_{x_2}^\dagger a_{x_3}^\dagger|\Omega\rangle\bigg) \tag{2.45}$$

for Θ_1 and Θ_3 as in (2.39). Finally, the coefficients $\psi_{N,\ell}$ in expansion (1.6) of the N-body ground state Ψ_N (Theorem 1) are constructed from this by inserting (2.42) into (2.7), i.e.,

$$\psi_{N,\ell} := \sum_{k=0}^{N}\varphi^{\otimes(N-k)}\otimes_s(\chi_\ell)^{(k)}. \tag{2.46}$$

The functions $\psi_{N,\ell}$ depend on N by construction. However, this N-dependence is trivial, since it comes only from the splitting into condensate φ and excitations χ. The coefficients χ_ℓ in expansion (1.6) of the excitations χ are completely independent of N.

2. Ground state energy

Another consequence of Proposition 2.1 is expansion (1.7) of the ground state energy $\mathcal{E}_N$ (Theorem 1). The coefficients E_ℓ in (1.7) are given as

$$E_\ell := \sum_{\nu=1}^{2\ell}\sum_{\substack{\boldsymbol{j}\in\mathbb{N}^\nu\\ |\boldsymbol{j}|=2\ell}}\sum_{\substack{\boldsymbol{m}\in\mathbb{N}_0^{\nu-1}\\ |\boldsymbol{m}|=\nu-1}}\frac{1}{\kappa(\boldsymbol{m})}\operatorname{Tr}\mathbb{P}_0\mathbb{H}_{j_1}\mathbb{O}_{m_1}\cdots\mathbb{H}_{j_{\nu-1}}\mathbb{O}_{m_{\nu-1}}\mathbb{H}_{j_\nu} \tag{2.47}$$

for $\mathbb{P}_0$ as in (2.26), $\mathbb{H}_j$ as in (2.23), $\mathbb{O}_m$ as in (2.37) and where

$$\kappa(\boldsymbol{m}) := 1 + |\{\mu : m_\mu = 0\}| \in \{1, \ldots, \nu - 1\} \tag{2.48}$$

is the number of operators $\mathbb{P}_0$ within the trace. This confirms the predictions of (formal) Rayleigh–Schrödinger perturbation theory. For example, the first coefficient in (2.47) simplifies to

$$E_1 = \langle \chi_0, \mathbb{H}_2 \chi_0 \rangle + \left\langle \chi_0, \mathbb{H}_1 \frac{\mathbb{Q}_0}{E_0 - \mathbb{H}_0} \mathbb{H}_1 \chi_0 \right\rangle. \tag{2.49}$$

3. Ground state reduced density

Finally, Proposition 2.1 implies an asymptotic expansion of the one-body reduced density $\gamma_N^{(1)}$ of Ψ_N (Corollary 1.1). The coefficients in (1.9) are given by the trace class operators with kernels

$$\gamma_{1,0}(x;y) := \varphi(x)\varphi(y), \tag{2.50a}$$

$$\begin{aligned}\gamma_{1,\ell}(x;y) := &\sum_{n=0}^{\ell-1}\sum_{k=0}^{\ell-n-1} \widetilde{c}_{\ell-n-1,k}\Big(\varphi(x)\operatorname{Tr}\mathbb{P}_{2n+1}a_y^\dagger(\mathcal{N}_{\perp\varphi}-1)^k + \varphi(y)\operatorname{Tr}\mathbb{P}_{2n+1}(\mathcal{N}_{\perp\varphi}-1)^k a_x\Big)\\ &+\sum_{n=0}^{\ell-1}\widetilde{c}_{\ell-n-1}\Big(\operatorname{Tr}\mathbb{P}_{2n}a_y^\dagger a_x - \varphi(x)\varphi(y)\operatorname{Tr}\mathbb{P}_{2n}\mathcal{N}_{\perp\varphi}\Big),\end{aligned} \tag{2.50b}$$

with

$$\widetilde{c}_\ell := (-1)^\ell c_\ell^{(3/2)}, \qquad \widetilde{c}_{\ell,k} := \widetilde{c}_{\ell-k} c_k^{(0)} \tag{2.51}$$

for $c_j^{(n)}$ as in (2.24a). For example, the leading order is $\gamma_{1,0} = p^\varphi$, which recovers the well-known fact that the ground state exhibits BEC with optimal rate. The first correction to this is given by

$$\begin{aligned}\gamma_{1,1}(x;y) &= \varphi(x)\operatorname{Tr}\mathbb{P}_1 a_y^\dagger + \varphi(y)\operatorname{Tr}\mathbb{P}_1 a_x\\ &\quad + \operatorname{Tr}\mathbb{P}_0 a_y^\dagger a_x - \varphi(x)\varphi(y)\operatorname{Tr}\mathbb{P}_0\mathcal{N}_{\perp\varphi}.\end{aligned} \tag{2.52}$$

For the ground state of a homogeneous Bose gas on the torus, $\gamma_{1,1}$ was recently derived in Ref. 10 using different methods. In that case, the first line in (2.52) vanishes by translation invariance. We prove Corollary 1.1 in Sec. II D.

C. Strategy of proof

The first step is to express $\mathbb{P}$ and $\mathbb{P}_0$ as contour integrals around the resolvents of $\mathbb{H}$ and $\mathbb{H}_0$, respectively, i.e.,

$$\mathbb{P} = \frac{1}{2\pi \mathrm{i}}\oint_\gamma \frac{1}{z - \mathbb{H}}\mathrm{d}z, \qquad \mathbb{P}_0 = \frac{1}{2\pi \mathrm{i}}\oint_\gamma \frac{1}{z - \mathbb{H}_0}\mathrm{d}z. \tag{2.53}$$

The contour γ is chosen such that its length is $\mathcal{O}(1)$ and that it encloses both the ground state energy $E_{\le N}$ of $\mathbb{H}_{\le N}$ and the Bogoliubov ground state energy E_0 but leaves the remaining spectra of $\mathbb{H}$ and $\mathbb{H}_0$ outside. Since $E_{\le N}$ converges to E_0 as $N \to \infty$ by (2.27), such a contour exists if the constant c in $\mathbb{H} = \mathbb{H}_{\le N} \oplus c$ from (2.19) is chosen a finite distance away from the spectrum of $\mathbb{H}_0$. This implies that $\mathbb{H}$ has precisely one (infinitely degenerate) additional eigenvalue c compared to $\mathbb{H}_{\le N}$. For simplicity, we place c at some finite distance below E_0 (see Fig. 1).

The next step is to expand $\mathbb{H}$ as[11]

$$\mathbb{H} = \sum_{j=0}^{a} \lambda_N^{\frac{j}{2}} \mathbb{H}_j + \lambda_N^{\frac{a+1}{2}} \mathbb{R}_a, \tag{2.54}$$

with $\mathbb{H}_j$ as in (2.23). The remainders $\mathbb{R}_a$, which are essentially the remainders of the Taylor series expansion of the square roots in (2.14), can be bounded above by powers of the number operator. Making use of expansion (2.54), we expand the resolvent of $\mathbb{H}$ around the resolvent of $\mathbb{H}_0$ and integrate along the contour γ, which finally yields

$$\mathbb{P} = \sum_{\ell=0}^{a} \lambda_N^{\frac{\ell}{2}} \mathbb{P}_\ell + \lambda_N^{\frac{a+1}{2}} \left(\mathbb{B}_P(a) + \mathbb{B}_Q(a)\right) \tag{2.55}$$

for $\mathbb{P}_\ell$ as in (2.36) and where

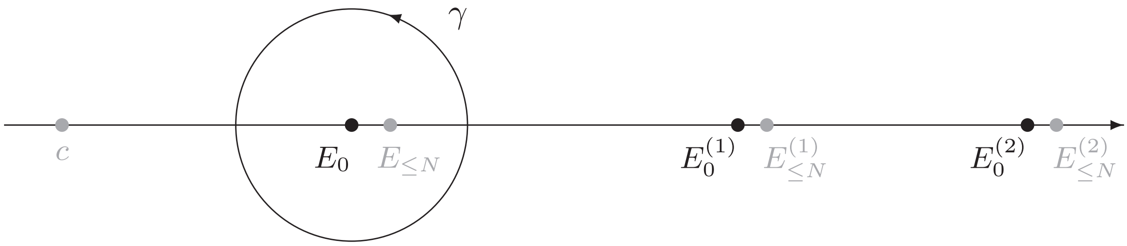

FIG. 1. Low-energy spectra of $\mathbb{H}_0$ (drawn in black) and $\mathbb{H}$ (drawn in gray). The additional eigenvalue c of $\mathbb{H}$ is placed a finite distance below E_0. For sufficiently large N, the contour γ around E_0 encloses the ground state energy $E_{\le N}$ of $\mathbb{H}_{\le N}$.

$$\mathbb{B}_P(a) = \sum_{\nu=0}^{a}\sum_{m=1}^{a-\nu}\sum_{\substack{j\in\mathbb{N}^m\\ |j|=a-\nu}} \frac{1}{2\pi \mathrm{i}}\oint_\gamma \frac{\mathbb{P}}{z-\mathbb{H}^<}\mathbb{R}_\nu \frac{1}{z-\mathbb{H}_0}\mathbb{H}_{j_1}\frac{1}{z-\mathbb{H}_0}\cdots\mathbb{H}_{j_m}\frac{1}{z-\mathbb{H}_0}\mathrm{d}z \tag{2.56}$$

and

$$\mathbb{B}_Q(a) = \sum_{\nu=0}^{a}\sum_{m=1}^{a-\nu}\sum_{\substack{j\in\mathbb{N}^m\\ |j|=a-\nu}}\sum_{\ell=0}^{m}\sum_{\substack{k\in\{0,1\}^{m+1}\\ |k|=\ell}} \frac{1}{2\pi \mathrm{i}}\oint_\gamma \frac{\mathbb{Q}}{z-\mathbb{H}^<}\mathbb{R}_\nu \frac{\mathbb{I}_{k_1}}{z-\mathbb{H}_0}\mathbb{H}_{j_1}\cdots\mathbb{H}_{j_m}\frac{\mathbb{I}_{k_{m+1}}}{z-\mathbb{H}_0}\mathrm{d}z \tag{2.57}$$

for $\mathbb{I}_k = \mathbb{P}_0$ if $k = 0$ and $\mathbb{I}_k = \mathbb{Q}_0$ if $k = 1$. To control the error terms, we estimate the operators $\mathbb{H}_j$ and $\mathbb{R}_\nu$ in terms of powers of $(\mathcal{N}_{\perp\varphi} + 1)$, prove a uniform bound on moments of the number operator with respect to $\boldsymbol{\chi}$, i.e.,

$$\left\langle \boldsymbol{\chi}, (\mathcal{N}_{\perp\varphi}+1)^b \boldsymbol{\chi}\right\rangle \le C(b), \tag{2.58}$$

and control alternating products of number operators and resolvents of $\mathbb{H}_0$ by means of the estimate

$$\left\| (\mathcal{N}_{\perp\varphi}+1)^{b+1}\frac{1}{z-\mathbb{H}_0}\boldsymbol{\phi}\right\| \le C(b)\|(\mathcal{N}_{\perp\varphi}+1)^b\boldsymbol{\phi}\|. \tag{2.59}$$

To derive expansion (2.61) of the ground state energy, we observe that

$$\mathrm{Tr}\,\mathbb{H}\mathbb{P} = \frac{1}{2\pi\mathrm{i}}\mathrm{Tr}\oint_\gamma\frac{\mathbb{H}}{z-\mathbb{H}}\mathrm{d}z = E_0 + \frac{1}{2\pi\mathrm{i}}\mathrm{Tr}\oint_\gamma\frac{z-E_0}{z-\mathbb{H}}\mathrm{d}z \tag{2.60}$$

and derive from this the expansion

$$\mathrm{Tr}\,\mathbb{H}\mathbb{P} = E_0 + \sum_{\ell=1}^{a}\lambda_N^{\frac{\ell}{2}}\sum_{\nu=1}^{\ell}\sum_{\substack{j\in\mathbb{N}^\nu\\ |j|=\ell}}\mathrm{Tr}\frac{1}{2\pi\mathrm{i}}\oint_\gamma\frac{1}{z-\mathbb{H}_0}\mathbb{H}_{j_1}\frac{1}{z-\mathbb{H}_0}\cdots\mathbb{H}_{j_\nu}\frac{z-E_0}{z-\mathbb{H}_0}\mathrm{d}z + \mathcal{O}\left(\lambda_N^{\frac{a+1}{2}}\right). \tag{2.61}$$

All half-integer powers of λ_N in (2.61) vanish by parity, which can be seen by conjugating with the unitary map $\mathcal{U}_P$ acting as $\mathcal{U}_P a^\dagger(f)\,\mathcal{U}_P = -a^\dagger(f)$ [recall from (2.23) that $\mathbb{H}_j$ contains an even/odd number of creation/annihilation operators for j even/odd]. After some lengthy computations, this yields (2.47).

D. Proof of corollary 1.1

To prove Corollary 1.1, one first observes that $\gamma_N^{(1)}$ can be decomposed as

$$\gamma_N^{(1)} = p^\varphi + \frac{1}{\sqrt{N}}(|\varphi\rangle\langle\beta_\chi| + |\beta_\chi\rangle\langle\varphi|) + \frac{1}{N}\left(\gamma_\chi - p^\varphi\,\mathrm{Tr}\,\mathbb{P}\mathcal{N}_{\perp\varphi}\right), \tag{2.62}$$

where γ_χ denotes the one-body reduced density matrix of $\boldsymbol{\chi}$ with kernel $\gamma_\chi(x;y) = \langle\boldsymbol{\chi}, a_y^\dagger a_x\boldsymbol{\chi}\rangle$ and where $\beta_\chi : \mathbb{R}^d \to \mathbb{C}$ is defined as

$$\beta_\chi(x) := \operatorname{Tr}\mathbb{P}\sqrt{1-\frac{\mathcal{N}_{\perp\varphi}}{N}}\,a_x \tag{2.63}$$

[see Ref. 2 (Sec. 3.5)]. Next, one expands the N-dependent expressions in (2.62) in powers of $\lambda_N^{1/2}$ and estimates the remainders using (a generalized version of) Proposition 2.1. We will show this for $a = 1$; the higher orders follow similarly using estimates from Ref. 1.

For $A \in \mathcal{L}(\mathfrak{H})$, (2.62) yields

$$\left|\operatorname{Tr}A\gamma_N^{(1)} - \operatorname{Tr}A\gamma_{1,0} - \lambda_N \operatorname{Tr}A\gamma_{1,1}\right| \le \left|\operatorname{Tr}\mathbb{P}a^\dagger(A\varphi)\frac{\sqrt{N-\mathcal{N}_{\perp\varphi}}}{N} - \lambda_N\operatorname{Tr}\mathbb{P}_1 a^\dagger(A\varphi)\right| \tag{2.64a}$$

$$+\left|\operatorname{Tr}\mathbb{P}\frac{\sqrt{N-\mathcal{N}_{\perp\varphi}}}{N}a(A\varphi) - \lambda_N\operatorname{Tr}\mathbb{P}_1 a(A\varphi)\right| \tag{2.64b}$$

$$+\left|\frac{1}{N}\operatorname{Tr}\mathrm{d}\Gamma(A)\mathbb{P} - \lambda_N\operatorname{Tr}\mathrm{d}\Gamma(A)\mathbb{P}_0\right| \tag{2.64c}$$

$$+|\langle\varphi, A\varphi\rangle|\left|\frac{1}{N}\operatorname{Tr}\mathbb{P}\mathcal{N}_{\perp\varphi} - \lambda_N\operatorname{Tr}\mathbb{P}_0\mathcal{N}_{\perp\varphi}\right|. \tag{2.64d}$$

In the first line, we expand $\sqrt{N-\mathcal{N}_{\perp\varphi}}/N = \lambda_N^{1/2} + \lambda_N^{3/2}\mathbb{R}$, where $\mathbb{R}$ is a function of $\mathcal{N}_{\perp\varphi}$ such that $\|\mathbb{R}\phi\| \lesssim \|(\mathcal{N}_{\perp\varphi}+1)\phi\|$ for any $\phi \in \mathcal{F}$ [see Ref. 2, Sec. 5H, Eq. (5-64b)]. By parity,

$$\operatorname{Tr}\mathbb{P}_0 a^\dagger(A\varphi)\mathbb{R} = \operatorname{Tr}\mathbb{P}_0 a^\dagger(A\varphi) = 0, \tag{2.65}$$

and hence,

$$\begin{aligned}(2.64\text{a}) \le \lambda_N^{\frac{1}{2}}&\left|\operatorname{Tr}\mathbb{P}a^\dagger(A\varphi) - \operatorname{Tr}\left(\mathbb{P}_0 + \lambda_N^{\frac{1}{2}}\mathbb{P}_1\right)a^\dagger(A\varphi)\right| \\ &+\lambda_N^{\frac{3}{2}}\left|\operatorname{Tr}\mathbb{P}a^\dagger(A\varphi)\mathbb{R} - \operatorname{Tr}\mathbb{P}_0 a^\dagger(A\varphi)\mathbb{R}\right|.\end{aligned} \tag{2.66}$$

Since

$$\|a^\dagger(A\varphi)\mathbb{R}\phi\| \le \|A\|_{\mathrm{op}}\|(\mathcal{N}_{\perp\varphi}+1)^{\frac{3}{2}}\phi\|, \qquad \|a^\dagger(A\varphi)\phi\| \le \|A\|_{\mathrm{op}}\|(\mathcal{N}_{\perp\varphi}+1)^{\frac{1}{2}}\phi\|, \tag{2.67}$$

one shows as in the proof of [Ref. 1 (Theorem 1)] that (2.66) $\lesssim \lambda_N^2\|A\|_{\mathrm{op}}$. The estimate of (2.64b) works analogously. For the third line in (2.64), one notes that $|1/N - \lambda_N| \lesssim \lambda_N^2$ and that $\operatorname{Tr}\mathbb{P}_1\mathrm{d}\Gamma(A) = 0$ by parity, and hence,

$$(2.64\text{c}) \lesssim \lambda_N^2|\operatorname{Tr}A\gamma_\chi| + \lambda_N\left|\operatorname{Tr}\left(\mathbb{P} - \mathbb{P}_0 - \lambda_N^{\frac{1}{2}}\mathbb{P}_1\right)\mathrm{d}\Gamma(A)\right| \lesssim \lambda_N^2\|A\|_{\mathrm{op}} \tag{2.68}$$

as above, where we used that $\|\mathrm{d}\Gamma(A)\phi\| \le \|A\|_{\mathrm{op}}\|(\mathcal{N}_{\perp\varphi}+1)\phi\|$ for any $\phi \in \mathcal{F}$. Analogously, we derive the bound $(2.64d) \lesssim \lambda_N^2\|A\|_{\mathrm{op}}$, making use of the fact that finite moments of $\mathcal{N}_{\perp\varphi}$ with respect to χ_0 and χ are bounded uniformly in N Ref. 1 [Lemmas 4.7(d) and 5.6(a)]. This concludes the proof of Corollary 1.1 by duality of compact and trace class operators. □

E. Extensions

The results proven in Ref. 1 are more general than what we have presented so far. In this section, we briefly comment on some extensions of Theorem 1.

1. Unbounded interaction potentials

One extension concerns unbounded interaction potentials, including the three-dimensional repulsive Coulomb potential. In fact, we can replace Assumption 1 by the following assumption:

Assumption 1'. Let $v : \mathbb{R}^d \to \mathbb{R}$ be measurable with $v(-x) = v(x)$ and $v \not\equiv 0$, and assume that there exists a constant $C > 0$ such that in the sense of operators on $\mathcal{Q}(-\Delta) = H^1(\mathbb{R}^d)$,

$$|v|^2 \le C(1-\Delta). \tag{2.69}$$

In addition, assume that v is of positive type.

In this situation, we require one additional assumption, ensuring that the N-body state exhibits complete BEC with not too many particles outside the condensate.

Assumption 3. Assume that there exist constants $C_1 \geq 0$, $0 < C_2 \leq 1$, and a function $\varepsilon : \mathbb{N} \to \mathbb{R}_0^+$ with

$$\lim_{N\to\infty} N^{-\frac{1}{3}} \varepsilon(N) \leq C_1$$

such that

$$H_N - N e_{\mathrm{H}} \geq C_2 \sum_{j=1}^{N} h_j - \varepsilon(N) \tag{2.70}$$

in the sense of operators on $\mathcal{D}(H_N)$.

Under these more general assumptions, several new issues arise, at the core of which is the problem that $\mathrm{d}\Gamma(v)$ cannot be bounded by powers of $\mathcal{N}_{\perp\varphi} + 1$ alone. This affects the Proof of Proposition 2.1 at multiple points; most notably, it becomes considerably more difficult to obtain the uniform bound on moments of the number operator (2.58).

2. Excited states

The analysis in Ref. 1 extends to the low-energy eigenstates of H_N, i.e., it includes all eigenstates with an energy of order one above the ground state energy. In this situation, the expansion must be done more carefully, since the excited eigenvalues $E_0^{(n)} > E_0$ of $\mathbb{H}_0$ can be degenerate, and the degeneracy of eigenvalues of $\mathbb{H}_{\leq N}$ may change in the limit $N \to \infty$. For instance, an eigenvalue $E_0^{(n)}$ of $\mathbb{H}_0$ could be twice degenerate, with two distinct eigenvalues $E_{\leq N}^{(n_1)} \neq E_{\leq N}^{(n_2)}$ of $\mathbb{H}_{\leq N}$ such that

$$\lim_{N\to\infty} E_{\leq N}^{(n_1)} = E_0^{(n)} = \lim_{N\to\infty} E_{\leq N}^{(n_2)}.$$

In this case, we expand the projector

$$\mathbb{P}^{(n)} = \frac{1}{2\pi\mathrm{i}} \oint_{\gamma^{(n)}} \frac{1}{z - \mathbb{H}} \mathrm{d}z \tag{2.71}$$

around

$$\mathbb{P}_0^{(n)} = \frac{1}{2\pi\mathrm{i}} \oint_{\gamma^{(n)}} \frac{1}{z - \mathbb{H}_0} \mathrm{d}z, \tag{2.72}$$

where $\gamma^{(n)}$ is a $\mathcal{O}(1)$ contour around $E_0^{(n)}$ with a finite distance to the remaining spectrum of $\mathbb{H}_0$. Since $\gamma^{(n)}$ encloses both poles $E_{\leq N}^{(n_1)}$ and $E_{\leq N}^{(n_2)}$ of $(z - \mathbb{H})^{-1}$, the contour integral (2.71) gives precisely the sum of the two spectral projectors of $\mathbb{H}$ corresponding to $E_{\leq N}^{(n_1)}$ and $E_{\leq N}^{(n_2)}$.

In Ref. 1, we show that there is a constant $C(a,n)$, which, in particular, depends on $|E_0^{(n)}|$, such that

$$\left| \mathrm{Tr}\, \mathbb{A}\mathbb{P}^{(n)} - \sum_{\ell=0}^{a} \lambda_N^{\frac{\ell}{2}} \mathrm{Tr}\, \mathbb{A}\mathbb{P}_\ell^{(n)} \right| \leq C(a,n) \lambda_N^{\frac{a+1}{2}} \|\mathbb{A}\|_{\mathrm{op}} \tag{2.73}$$

for sufficiently large N. The coefficients $\mathbb{P}_\ell^{(n)}$ are defined analogously to $\mathbb{P}_\ell$ from (2.36) but with $\mathbb{P}_0$ replaced by $\mathbb{P}_0^{(n)}$. Note that the statement is non-trivial only for states with an energy of order one above the ground state energy because the constant $C(a,n)$ depends on $|E_0|$.

To state the generalization of expansion (1.7) to the low-energy spectrum of H_N, we need some more notation. We denote by

$$\mathscr{E}_N \equiv \mathscr{E}_N^{(0)} < \mathscr{E}_N^{(1)} < \cdots < \mathscr{E}_N^{(\nu)} < \cdots$$

the eigenvalues of H_N and by $\delta_N^{(\nu)}$ the degeneracy of $\mathscr{E}_N^{(\nu)}$ (we follow the convention of counting eigenvalues without multiplicity). Given an eigenvalue $E_0^{(n)}$ of $\mathbb{H}_0$, we collect the indices ν of the eigenvalues $\mathscr{E}_N^{(\nu)}$ that converge to $Ne_{\mathrm{H}} + E_0^{(n)}$ for some given n in the index set

$$\iota^{(n)} := \left\{ \nu \in \mathbb{N}_0 : \lim_{N\to\infty} \left(\mathscr{E}_N^{(\nu)} - Ne_{\mathrm{H}} \right) = E_0^{(n)} \right\}. \tag{2.74}$$

The generalization of (1.7) to excited eigenvalues $\mathscr{E}_N^{(n)}$ is then given by

$$\left| \sum_{\nu \in \iota^{(n)}} \delta_N^{(\nu)} \mathscr{E}_N^{(\nu)} - \delta_0^{(n)} N e_{\mathrm{H}} - \sum_{\ell=0}^{a} \lambda_N^{\ell} E_\ell^{(n)} \right| \le C(a,n) \lambda_N^{a+1}, \tag{2.75}$$

where $\delta_0^{(n)}$ denotes the degeneracy of $E_0^{(n)}$ and where $E_\ell^{(n)}$ is defined as in (2.47) but with $\mathbb{P}_0$ replaced by $\mathbb{P}_0^{(n)}$. The constant $C(a,n)$ depends on $|E_0^{(n)}|$.

3. Expectation values of unbounded operators

Finally Ref. 1 yields an asymptotic expansion of expectation values of self-adjoint m-body operators $A^{(m)}$, which are relatively bounded with respect to $\sum_{j=1}^m (-\Delta_j + V(x_j))$, i.e.,

$$\|A^{(m)}\psi\|_{\mathfrak{H}^m} \le \mathfrak{C} \left\| \sum_{j=1}^m (-\Delta_j + V(x_j) + 1)\psi \right\|_{\mathfrak{H}^m} \qquad \text{for } \psi \in \mathcal{D}\left(\sum_{j=1}^m (-\Delta_j + V(x_j)) \right). \tag{2.76}$$

For $\mathcal{A}_N^{(m)}$, the symmetrized version of $A^{(m)}$,

$$\mathcal{A}_N^{(m)} := \binom{N}{m}^{-1} \sum_{1\le j_1 < \cdots < j_m \le N} A^{(m)}_{j_1,\ldots,j_m}, \tag{2.77}$$

we prove that there exists a constant $C(m,a)$ such that

$$\left| \left\langle \Psi_N, \mathcal{A}_N^{(m)} \Psi_N \right\rangle - \sum_{\ell=0}^{a} \lambda_N^{\frac{\ell}{2}} \mathrm{Tr}\left((\mathfrak{U}_{N,\varphi} \mathcal{A}_N^{(m)} \mathfrak{U}_{N,\varphi}^* \oplus 0) \mathbb{P}_\ell^{(n)} \right) \right| \le C(m,a) \lambda_N^{\frac{a+2}{2}} \tag{2.78}$$

for sufficiently large N. The statement extends to excited states as explained in Sec. II E 2.

The rate in (2.78) is by a factor $\lambda_N^{1/2}$ better than the error estimate in Proposition 2.1. To see this, one considers the operator

$$\mathbb{A}_{\mathrm{red}}^{(m)} = \mathfrak{U}_{N,\varphi} \left(\mathcal{A}_N^{(m)} - \left\langle \varphi^{\otimes N}, \mathcal{A}_N^{(m)} \varphi^{\otimes N} \right\rangle \right) \mathfrak{U}_{N,\varphi}^* \oplus 0,$$

where we have subtracted the condensate expectation value of $\mathcal{A}_N^{(m)}$ (which is of order one). Because of this subtraction, one can show that $\mathbb{A}_{\mathrm{red}}^{(m)}$ satisfies the estimate

$$\|\mathbb{A}_{\mathrm{red}}^{(m)} \phi\|_{\mathcal{F}_{\perp\varphi}} \lesssim \lambda_N^{\frac{1}{2}}, \qquad \Phi \in \{\chi, \chi_0\}, \tag{2.79}$$

and Proposition 2.1 for $\mathbb{A}_{\mathrm{red}}^{(m)}$ concludes the proof.

III. DYNAMICS

In the remaining part of this Review, we study the dynamics generated by the Hamiltonian H_N from (1.4) and explain expansions (1.10) and (1.12) of the time-evolved N-body wave function Ψ_N and of the reduced one-body density $\gamma_N^{(1)}$. We use the superscript$^{\mathrm{trap}}$ wherever it applies.

A. Framework

We study the solutions $\Psi_N(t)$ of the time-dependent N-body Schrödinger equation (1.3) generated by the Hamiltonian H_N from (1.4), which describes a system of N interacting bosons without an external trapping potential. As the initial state, we take

$$\Psi_N(0) = \Psi_N^{\mathrm{trap}},$$

where Ψ_N^{trap} is the ground state of H_N^{trap}.

1. Condensate

As explained above, Ψ_N^{trap} exhibits BEC in the Hartree minimizer φ^{trap}, and it is well known that this property is preserved by the time evolution. More precisely,

$$\mathrm{Tr}\left| \gamma_N^{(1)}(t) - |\varphi(t)\rangle\langle\varphi(t)| \right| \le \frac{C(t)}{N} \tag{3.1}$$

(see, e.g., Refs. 12 and 13), where $\varphi(t)$ is the solution of the Hartree equation,

$$\mathrm{i}\partial_t\varphi(t) = \left(-\Delta + v * |\varphi(t)|^2 - \mu^{\varphi(t)}\right)\varphi(t) =: h^{\varphi(t)}\varphi(t), \qquad \varphi(0) = \varphi^{\mathrm{trap}}, \tag{3.2}$$

with the phase factor $\mu^{\varphi(t)} = \frac{1}{2}\int_{\mathbb{R}^d}\left(v * |\varphi(t)|^2\right)(x)|\varphi(t,x)|^2\mathrm{d}x$. The solution of (3.2) in $H^1(\mathbb{R}^d)$ is unique and exists globally. We define the projectors $p^{\varphi(t)}$ and $q^{\varphi(t)}$ analogously to (2.3).

2. Excitations

Analogously to (2.7), we decompose the time-evolved N-body state $\Psi_N(t)$ into the condensate $\varphi(t)$ and excitations $\chi_{\leq N}(t)$ from the condensate. The excitation vector $\chi_{\leq N}(t)$ is an element of the (truncated) excitation Fock space $\mathcal{F}^{\leq N}_{\perp\varphi(t)} \subset \mathcal{F}_{\perp\varphi(t)} \subset \mathcal{F}$ defined analogously to (2.9). When restricted to the time-dependent excitation Fock space $\mathcal{F}_{\perp\varphi(t)}$, the number operator $\mathcal{N}$ on the (time-independent) Fock space $\mathcal{F}$ counts the number of excitations around the time-evolved condensate $\varphi(t)^{\otimes N}$. As before, the relation between $\Psi_N(t)$ and $\chi_{\leq N}(t)$ is given by the (now time-dependent) unitary map $\mathfrak{U}_{N,\varphi(t)}$ defined analogously to (2.11), namely,

$$\chi_{\leq N}(t) = \mathfrak{U}_{N,\varphi(t)}\Psi_N(t). \tag{3.3}$$

The evolution of the excitations is determined by the Schrödinger equation

$$\mathrm{i}\partial_t\chi_{\leq N}(t) = \mathbb{H}^{\varphi(t)}_{\leq N}\chi_{\leq N}(t), \qquad \chi_{\leq N}(0) = \mathfrak{U}_{N,\varphi^{\mathrm{trap}}}\Psi^{\mathrm{trap}}_N \tag{3.4}$$

on $\mathcal{F}^{\leq N}_{\perp\varphi(t)}$, generated by the excitation Hamiltonian

$$\mathbb{H}^{\varphi(t)}_{\leq N} = \mathrm{i}(\partial_t\mathfrak{U}_{N,\varphi(t)})\mathfrak{U}^*_{N,\varphi(t)} + \mathfrak{U}_{N,\varphi(t)}H_N\mathfrak{U}^*_{N,\varphi(t)}. \tag{3.5}$$

For convenience, we write $\mathbb{H}^{\varphi(t)}_{\leq N}$ as restriction to $\mathcal{F}^{\leq N}_{\perp\varphi(t)}$ of a Hamiltonian $\mathbb{H}^{\varphi(t)}$ on $\mathcal{F}$, which can be expressed, analogously to (2.14), in terms of N, $\mathcal{N}$, and operators $\mathbb{K}^{\varphi(t)}_j$, which are defined analogously[14] to (2.15). Expanding the N-dependent expressions in a Taylor series yields (formally) the power series

$$\mathbb{H}^{\varphi(t)} = \mathbb{H}^{\varphi(t)}_0 + \sum_{n\geq 1}\lambda_N^{\frac{n}{2}}\mathbb{H}^{\varphi(t)}_n, \tag{3.6}$$

with coefficients $\mathbb{H}^{\varphi(t)}_j$ analogously to (2.23). Note that the operator $\mathbb{H}^{\varphi(t)}$ preserves the truncation of $\mathcal{F}^{\leq N}$, whereas this property is lost when truncating the expansion after finitely many terms.

3. Bogoliubov approximation

The leading order $\mathbb{H}^{\varphi(t)}_0$ in (3.6) is the time-dependent Bogoliubov Hamiltonian, which generates the Bogoliubov time evolution,

$$\mathrm{i}\partial_t\chi_0(t) = \mathbb{H}^{\varphi(t)}_0\chi_0(t), \qquad \chi_0(0) = \chi_0^{\mathrm{trap}}. \tag{3.7}$$

It is well known that the solution of (3.7) approximates the solution $\chi_{\leq N}(t)$ of (3.4) to leading order, i.e.,

$$\lim_{N\to\infty}\|\chi_{\leq N}(t) - \chi_0(t)\|_{\mathcal{F}^{\leq N}_{\perp\varphi(t)}} = 0 \tag{3.8}$$

(see, e.g., Refs. 15 and 16). This is a very useful approximation because the time evolution generated by $\mathbb{H}^{\varphi(t)}_0$ acts as a Bogoliubov transformation $\mathbb{U}_{\mathcal{V}(t,s)}$ on $\mathcal{F}$. This means a huge simplification compared with the full N-body dynamics because it essentially reduces the N-body problem to the problem of solving a 2×2 matrix differential equation: the corresponding Bogoliubov map $\mathcal{V}(t,s)$ on $\mathfrak{H}\oplus\mathfrak{H}$ is determined by the differential equation

$$\mathrm{i}\partial_t\mathcal{V}(t,s) = \mathcal{A}(t)\mathcal{V}(t,s), \qquad \mathcal{V}(s,s) = \mathbb{1}, \tag{3.9}$$

with

$$\mathcal{V}(t,s) = \begin{pmatrix} U_{t,s} & \overline{V}_{t,s} \\ V_{t,s} & \overline{U}_{t,s}\end{pmatrix}, \qquad \mathcal{A}(t) = \begin{pmatrix} h^{\varphi(t)} + K_1^{\varphi(t)} & -K_2^{\varphi(t)} \\ \overline{K_2^{\varphi(t)}} & -\left(\overline{h^{\varphi(t)} + K_1^{\varphi(t)}}\right)\end{pmatrix}. \tag{3.10}$$

Since it is a Bogoliubov transformation, the Bogoliubov time evolution preserves quasi-freeness. Hence, $\chi_0(t)$ is uniquely determined by its two-point functions,

$$\gamma_{\chi_0(t)}(x,y) = \left\langle \chi_0(t), a_y^\dagger a_x \chi_0(t)\right\rangle_{\mathcal{F}}, \qquad \alpha_{\chi_0(t)}(x,y) = \left\langle \chi_0(t), a_x a_y \chi_0(t)\right\rangle_{\mathcal{F}}, \tag{3.11}$$

which can be computed directly from the two-point functions of $\chi_0(0)$ as

$$\gamma_{\chi_0(t)}(x,y) = \left(\overline{V}_{t,0}\gamma^T_{\chi_0(0)}\overline{V}^*_{t,0} + U_{t,0}\gamma_{\chi_0(0)}U^*_{t,0} - \overline{V}_{t,0}\alpha^*_{\chi_0(0)}U^*_{t,0} - U_{t,0}\alpha_{\chi_0(0)}\overline{V}^*_{t,0}\right)(x,y) + \left(\overline{V}_{t,0}\overline{V}^*_{t,0}\right)(x,y), \tag{3.12a}$$

$$\alpha_{\chi_0(t)}(x,y) = \left(U_{t,0}\alpha_{\chi_0(0)}\overline{U}^*_{t,0} + \overline{V}_{t,0}\alpha^*_{\chi_0(0)}V^*_{t,0} - U_{t,0}\gamma_{\chi_0(0)}V^*_{t,0} - \overline{V}_{t,0}\gamma^T_{\chi_0(0)}\overline{U}^*_{t,0}\right)(x,y) + \left(U_{t,0}V^*_{t,0}\right)(x,y). \tag{3.12b}$$

Alternatively, one obtains $\gamma_{\chi_0(t)}$ and $\alpha_{\chi_0(t)}$ by solving the system of differential equations

$$\mathrm{i}\partial_t\gamma_{\chi_0(t)} = \left(h^{\varphi(t)} + K_1^{\varphi(t)}\right)\gamma_{\chi_0(t)} - \gamma_{\chi_0(t)}\left(h^{\varphi(t)} + K_1^{\varphi(t)}\right) + K_2^{\varphi(t)}\alpha^*_{\chi_0(t)} - \alpha_{\chi_0(t)}\left(K_2^{\varphi(t)}\right)^*, \tag{3.13a}$$

$$\mathrm{i}\partial_t\alpha_{\chi_0(t)} = \left(h^{\varphi(t)} + K_1^{\varphi(t)}\right)\alpha_{\chi_0(t)} + \alpha_{\chi_0(t)}\left(h^{\varphi(t)} + K_1^{\varphi(t)}\right)^T + K_2^{\varphi(t)} + K_2^{\varphi(t)}\gamma^T_{\chi_0(t)} + \gamma_{\chi_0(t)}K_2^{\varphi(t)} \tag{3.13b}$$

(see Refs. 16 and 17).

B. Expansion of the dynamics

1. Expansion of the time-evolved wave function

With the formal ansatz

$$\chi_{\le N}(t) \oplus 0 = \sum_{\ell=0}^{\infty} \lambda_N^{\frac{\ell}{2}}\chi_\ell(t), \tag{3.14}$$

the Schrödinger equation (3.4) leads to the set of equations

$$\mathrm{i}\partial_t\chi_\ell(t) = \mathbb{H}_0^{\varphi(t)}\chi_\ell(t) + \sum_{n=1}^{\ell}\mathbb{H}_n^{\varphi(t)}\chi_{\ell-n}(t). \tag{3.15}$$

Motivated by (3.15), we define iteratively

$$\chi_\ell(t) := \mathbb{U}_{\mathcal{V}(t,0)}\chi_\ell(0) - \mathrm{i}\sum_{n=1}^{\ell}\int_0^t \mathbb{U}_{\mathcal{V}(t,s)}\,\mathbb{H}_n^{\varphi(s)}\,\chi_{\ell-n}(s)\mathrm{d}s, \tag{3.16}$$

where $\mathbb{U}_{\mathcal{V}(t,s)}$ denotes the Bogoliubov time evolution, i.e., the Bogoliubov transformation corresponding to the solution $\mathcal{V}(t,s)$ of (3.9). To prove Theorem 2, we show that these functions χ_ℓ are the coefficients in an asymptotic expansion of $\chi_{\le N}$.

Proposition 3.1. Let Assumption 1a be satisfied, let $a \in \mathbb{N}_0$, and denote by $\chi_{\le N}(t)$ the solution of (3.4). Then, $\chi_\ell(t) \in \mathcal{F}_{\perp\varphi(t)}$ and there exists a constant $C(a)$ such that

$$\left\|\chi_{\le N}(t) - \sum_{\ell=0}^{a}\lambda_N^{\frac{\ell}{2}}\chi_\ell(t)\right\|_{\mathcal{F}^{\le N}} \le \mathrm{e}^{C(a)t}\lambda_N^{\frac{a+1}{2}} \tag{3.17}$$

for all $t \in \mathbb{R}$ and sufficiently large N.

The growth of the constant $C(a)$ in a can be estimated as

$$C(a) \le Ca^2 \ln a. \tag{3.18}$$

We do not expect this to be optimal, especially since Borel summability was shown for a comparable expansion in Ref. 18. As a consequence of Proposition 3.1, the coefficients $\Psi_{N,\ell}(t)$ of expansion (1.10) of $\Psi_N(t)$ are given by

$$\Psi_{N,\ell}(t) := \sum_{k=0}^{N} \varphi(t)^{\otimes(N-k)} \otimes_s (\chi_\ell(t))^{(k)}. \tag{3.19}$$

The higher orders $\chi_\ell(t)$ are completely determined by the solution $\chi_0(t)$ of the Bogoliubov equation as

$$\chi_\ell(t) = \sum_{\substack{0,\le,n\le 3\ell \\ n+\ell \text{ even}}} \sum_{j\in\{-1,1\}^n} \int \mathrm{d}x^{(n)} \mathfrak{C}^{(j)}_{\ell,n}(t;x^{(n)})\ a^{\sharp_{j_1}}_{x_1} \cdots a^{\sharp_{j_n}}_{x_n} \chi_0(t), \tag{3.20}$$

where we used the notation

$$a^{\sharp_{-1}}_x := a_x, \qquad a^{\sharp_1}_x := a^\dagger_x. \tag{3.21}$$

The N-independent functions $\mathfrak{C}^{(j)}_{\ell,n}$ are given in terms the matrix entries $U_{t,s}$ and $V_{t,s}$ of the solution $\mathcal{V}(t,s)$ of (3.9) and the initial data. For example,

$$\mathfrak{C}^{(1)}_{1,1}(t) = \Big(U_{t,0}(U^{\text{trap}}_0)^* - \overline{V}_{t,0}(\overline{V^{\text{trap}}_0})^*\Big)\Theta^{\text{trap}}_1, \tag{3.22a}$$

$$\mathfrak{C}^{(-1)}_{1,1}(t) = \Big(V_{t,0}(U^{\text{trap}}_0)^* - \overline{U}_{t,0}(\overline{V^{\text{trap}}_0})^*\Big)\Theta^{\text{trap}}_1 \tag{3.22b}$$

for Θ^{trap}_1 as in (2.39). Here, U^{trap}_0 and V^{trap}_0 denote the matrix entries of the Bogoliubov map corresponding to the Bogoliubov transformation $\mathbb{U}^{\text{trap}}_{\mathcal{V}_0}$ that diagonalizes $\mathbb{H}^{\text{trap}}_0$. The coefficients $\mathfrak{C}^{(j)}_{\ell,n}$ with larger indices are constructed from this in a systematic iterative procedure. Since the general formula is very long and not particularly insightful, we refrain from stating it here and refer to Ref. 2 [Eq. (5.51)].

The higher orders $\chi_\ell(t)$ satisfy a generalized Wick rule for the "mixed" correlation functions,

$$\Big\langle a^{\sharp_1}_{x_1}\cdots a^{\sharp_n}_{x_n}\Big\rangle^{(t)}_{\ell,k} := \Big\langle \chi_\ell(t), a^{\sharp_1}_{x_1}\cdots a^{\sharp_n}_{x_n}\chi_k(t)\Big\rangle. \tag{3.23}$$

Proposition 3.2 (generalized Wick rule).

- *If $k+\ell+n$ odd,*

$$\Big\langle a^{\sharp_{j_1}}_{x_1}\cdots a^{\sharp_{j_n}}_{x_n}\Big\rangle^{(t)}_{\ell,k} = 0. \tag{3.24}$$

- *If $k+\ell+n$ even,*

$$\Big\langle a^{\sharp_{j_1}}_{x_1}\cdots a^{\sharp_{j_n}}_{x_n}\Big\rangle^{(t)}_{\ell,k} = \sum_{\substack{b=n\\ \text{even}}}^{n+3(\ell+k)} \sum_{m\in\{-1,1\}^b} \sum_{\sigma\in P_b} \prod_{i=1}^{b/2} \int \mathrm{d}y^{(b)} \mathfrak{D}^{(j;m)}_{\ell,k,n;b}(t;x^{(n)};y^{(b)}) \Big\langle a^{\sharp_{m_{\sigma(2i-1)}}}_{y_{\sigma(2i-1)}} a^{\sharp_{m_{\sigma(2i)}}}_{y_{\sigma(2i)}}\Big\rangle^{(t)}_{0,0} \tag{3.25}$$

for P_b being the set of pairings defined in (2.33). The functions $\mathfrak{D}^{(j;m)}_{\ell,k,n;b}$ are determined by the coefficients $\mathfrak{C}$ from (3.20) [see Ref. 2 (Corollary 3.5) for the precise formula].

2. Expansion of the one-body reduced density matrix

As an application of (3.17), we derive expansion (1.12) of the one-body reduced density matrix. The coefficients $\gamma^{(1)}_{N,\ell}$ in (1.12) are given by the trace class operators with kernels

$$\gamma_{1,0}(t;x;y) := \varphi(t,x)\overline{\varphi(t,y)}, \tag{3.26a}$$

$$\begin{aligned}\gamma_{1,\ell}(t;x;y) := \sum_{m=1}^{\ell}\Bigg[\sum_{k=0}^{\ell-m}\sum_{n=0}^{2m-1}\widetilde{c}_{\ell-m,k}\bigg(\varphi(t,x)\Big\langle a^\dagger_y(\mathcal{N}-1)^k\Big\rangle^{(t)}_{n,2m-n-1}\\ +\Big\langle(\mathcal{N}-1)^k a_x\Big\rangle^{(t)}_{n,2m-n-1}\overline{\varphi(t,y)}\bigg)\\ +\sum_{n=0}^{2m-2}\widetilde{c}_{\ell-m}\bigg(\Big\langle a^\dagger_y a_x\Big\rangle^{(t)}_{n,2m-n-2} - \varphi(t,x)\overline{\varphi(t,y)}\langle\mathcal{N}\rangle^{(t)}_{n,2m-n-2}\bigg)\Bigg],\end{aligned} \tag{3.26b}$$

with $\widetilde{c}_\ell$ and $\widetilde{c}_{\ell,k}$ as in (2.51) and where we used the notation (3.23). For example, the leading order of the expansion is $\gamma_0^{(1)}(t) = p^{\varphi(t)}$, which recovers (3.1). The next-to-leading order is given by

$$\gamma_1^{(1)}(t) = |\varphi(t)\rangle\langle\beta_{0,1}(t)| + |\beta_{0,1}(t)\rangle\langle\varphi(t)| + \gamma_{\chi_0(t)} - \operatorname{Tr}\gamma_{\chi_0(t)}p^{\varphi(t)}, \tag{3.27}$$

where the function $\beta_{0,1}:\mathbb{R}^d\to\mathbb{C}$ is the solution of

$$\begin{aligned} \mathrm{i}\partial_t\beta_{0,1}(t) &= \left(h^{\varphi(t)} + K_1^{\varphi(t)}\right)\beta_{0,1}(t) + K_2^{\varphi(t)}\overline{\beta_{0,1}(t)} \\ &\quad+\left(K_3^{\varphi(t)}\right)^*\alpha_{\chi_0(t)} + \operatorname{Tr}_1\left(K_3^{\varphi(t)}\gamma_{\chi_0(t)}\right) + \operatorname{Tr}_2\left(K_3^{\varphi(t)}\gamma_{\chi_0(t)}\right). \end{aligned} \tag{3.28}$$

Here, $\gamma_{\chi_0(t)}$ and $\alpha_{\chi_0(t)}$ are the Bogoliubov two-point functions as in (3.11), and we used the notation $\operatorname{Tr}_1 A := \int dz A(z,\cdot;\ z)$ and $\operatorname{Tr}_2 A := \int dz A(\cdot, z;\ z)$ for an operator $A:\mathfrak{H}\to\mathfrak{H}^2$.

C. Strategy of proof

To prove Proposition 3.1, we first show that the functions $\boldsymbol{\chi}_\ell(t)$ defined in (3.16) are elements of $\mathcal{F}_{\perp\varphi(t)}$ by proving that

$$\left\langle\boldsymbol{\chi}_\ell(t), (\mathcal{N}+1)^b\boldsymbol{\chi}_\ell(t)\right\rangle_{\mathcal{F}} \lesssim \mathrm{e}^{C(\ell,b)t} \tag{3.29}$$

for any $b\in\mathbb{N}_0$. To this end, we re-write $\boldsymbol{\chi}_\ell(t)$ as

$$\boldsymbol{\chi}_\ell(t) = \mathbb{U}_{\mathcal{V}(t,0)}\boldsymbol{\chi}_\ell(0) + \sum_{n=0}^{\ell-1}\sum_{m=1}^{\ell-n}\sum_{\substack{\boldsymbol{j}\in\mathbb{N}^m\\|\boldsymbol{j}|=\ell-n}}(-\mathrm{i})^m\int_0^t ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{m-1}}ds_m\,\widetilde{\mathbb{H}}_{t,s_1}^{(j_1)}\cdots\widetilde{\mathbb{H}}_{t,s_m}^{(j_m)}\,\mathbb{U}_{\mathcal{V}(t,0)}\boldsymbol{\chi}_n(0), \tag{3.30}$$

with

$$\widetilde{\mathbb{H}}_{t,s}^{(n)} := \mathbb{U}_{\mathcal{V}(t,s)}\mathbb{H}_n^{\varphi(s)}\,\mathbb{U}_{\mathcal{V}(t,s)}^*, \tag{3.31}$$

bound the operators $\widetilde{\mathbb{H}}_{t,s}^{(n)}$ by powers of $(\mathcal{N}+1)$, and make use of the fact that any finite moment of $\mathcal{N}$ with respect to $\boldsymbol{\chi}_n(0)$ is bounded since $\boldsymbol{\chi}_n(0) = \boldsymbol{\chi}_n^{\mathrm{trap}}$ from (2.42). To prove (3.17), we expand $\mathbb{H}^{\varphi(t)}$ in a Taylor series with remainder analogously to (2.54), prove an estimate the remainder in terms of $\mathcal{N}$, and make use of (3.29) to close a Gronwall argument for the function $\widetilde{\boldsymbol{\chi}}_a(t) = \boldsymbol{\chi}_{\le N}(t)\oplus 0 - \sum_{\ell=0}^a\lambda_N^{\ell/2}\boldsymbol{\chi}_\ell(t)$.

To prove Corollary 1.2, one decomposes $\gamma_N^{(1)}(t)$ analogously to (2.62) and expands it in powers of $\lambda_N^{1/2}$, which yields expressions containing correlation functions of $\boldsymbol{\chi}_{\le N}$,

$$\left\langle a_{x_1}^{\sharp_1}\cdots a_{x_n}^{\sharp_n}\right\rangle_N^{(t)} := \left\langle\boldsymbol{\chi}_{\le N}(t), a_{x_1}^{\sharp_1}\cdots a_{x_n}^{\sharp_n}\boldsymbol{\chi}_{\le N}(t)\right\rangle_{\mathcal{F}^{\le N}}. \tag{3.32}$$

Finally, we show that, in a suitable sense,

$$\left\langle a_{x_1}^{\sharp_1}\cdots a_{x_n}^{\sharp_n}\right\rangle_N^{(t)} = \sum_{\ell=0}^a\lambda_N^{\frac{\ell}{2}}\sum_{m=0}^{\ell}\left\langle\boldsymbol{\chi}_m(t), a_{x_1}^{\sharp_1}\cdots a_{x_n}^{\sharp_n}\boldsymbol{\chi}_{\ell-m}(t)\right\rangle_{\mathcal{F}} + \mathcal{O}\left(\lambda_N^{\frac{a+1}{2}}\right), \tag{3.33}$$

where all half-integer powers of λ_N vanish by the generalized Wick rule (Proposition 3.2).

D. Extensions

The results proven in Ref. 2 are more general than what was stated so far, namely, they admit a larger class of initial data. It is not necessary to start the time evolution in the ground state Ψ_N^{trap} of the trapped system (or in any low-energy eigenstate of H_N^{trap}), but it suffices if the initial state satisfies the following assumption:

Assumption 4. Let $\widetilde{a}\in\mathbb{N}_0$. *Let* $\Psi_N(0)\in\mathcal{D}(H_N)$, *define* $\boldsymbol{\chi}_{\le N}(0) = \mathfrak{U}_{N,\varphi(0)}\Psi_N(0)$, *and assume that there exists a constant* $C(\widetilde{a})>0$ *such that*

$$\left\|\boldsymbol{\chi}_{\le N}(0) - \sum_{\ell=0}^{\widetilde{a}}\lambda_N^{\frac{\ell}{2}}\boldsymbol{\chi}_\ell(0)\right\|_{\mathcal{F}^{\le N}} \le C(\widetilde{a})\,\lambda_N^{\frac{\widetilde{a}+1}{2}}, \tag{3.34}$$

where the functions $\chi_\ell(0)$ *are defined as follows:*

- *Let* $\widetilde{\nu} \in \mathbb{N}_0$, *let* $\mathbb{U}_{\mathcal{V}_0}$ *be a Bogoliubov transformation on* $\mathcal{F}_{\perp\varphi(0)}$, *and let* $\{f_j\}_{j=1}^{\widetilde{\nu}} \subset \{\varphi(0)\}^\perp$ *be some orthonormal system. Define*

$$\chi_0(0) := \mathbb{U}_{\mathcal{V}_0} a^\dagger(f_1) \cdots a^\dagger(f_{\widetilde{\nu}}) |\Omega\rangle. \tag{3.35}$$

- *For* $1 \le \ell \le \widetilde{a}$, *let*

$$\chi_\ell(0) = \sum_{\substack{0\le m\le 3\ell \\ m+\ell \text{ even}}} \sum_{\mu=0}^{m} \int \mathrm{d}x^{(\mu)} \mathrm{d}y^{(m-\mu)} \widetilde{\mathfrak{a}}_{m,\mu}^{(\ell)}\Big(x^{(\mu)}; y^{(m-\mu)}\Big) a_{x_1}^\dagger \cdots a_{x_\mu}^\dagger a_{y_1} \cdots a_{y_{m-\mu}} \chi_0(0), \tag{3.36}$$

where $\mathfrak{a}_{n,m,\mu}^{(\ell)}\Big(x^{(\mu)}; y^{(m-\mu)}\Big)$ *are the kernels of some N-independent bounded operators.*

Moreover, our analysis generalizes to the case where $\chi_0(0)$ is given as a linear combination of Bogoliubov transformed states with different particle numbers $\widetilde{\nu}$. It is clear that this is satisfied by any superposition of low-energy eigenstates of H_N^{trap}.

E. Related results

We conclude with a brief overview of closely related results in the literature. The first derivation of higher order corrections is due to Ginibre and Velo,[18,19] who consider the classical field limit $\hbar \to 0$ of the dynamics generated by a Hamiltonian on Fock space with coherent states as initial data. They construct a Dyson expansion of the unitary group $W(t,s)$ in terms of the time evolution generated by the Bogoliubov Hamiltonian; moreover, they prove that the expansion is Borel summable for bounded interaction potentials.[18] The main difference to our work (apart from the Fock space setting) is that the authors expand the time evolution operator $W(t,s)$ in a perturbation series (and not the wave function). In contrast, we derive an expansion of the time-evolved wave function for a specific, physically relevant choice of initial data. This simplifies the approximation since fewer terms are required at a given order of the approximation because the state is expanded simultaneously with the Hamiltonian.

Another approach to higher order corrections in the mean-field regime in the N-body setting was proposed by Paul and Pulvirenti.[20] In that work, the authors approach the problem from a kinetic theory perspective and consider the dynamics of the reduced density matrices of the N-body state. Their approach is formally similar to ours, since Bogoliubov theory in the sense of linearization of the Hartree equation is used for the expansion and an a-dependent but N-independent number of operations is required for the construction. In comparison, the main advantage of our approach is that the coefficients χ_ℓ in our approximation are completely independent of N.

Finally, a similar result in the N-body setting was obtained in a joint work with Pavlović, Pickl, and Soffer[21] In this paper, we expand the N-body time evolution in a Dyson series comparable to (3.16) but with one crucial difference: instead of using the Bogoliubov time evolution, the expansion is in terms of an auxiliary time evolution $\widetilde{U}_\varphi(t,s)$ on $\mathfrak{H}^N$, whose generator has a quadratic structure comparable to the Bogoliubov Hamiltonian (sometimes called the particle number preserving Bogoliubov Hamiltonian).

Unfortunately, this auxiliary time evolution $\widetilde{U}_\varphi(t,s)$ is a rather inaccessible object, which implicitly still depends on N. In particular, it is not clear to what extent computations are less complex with respect to the time evolution $\widetilde{U}_\varphi(t,s)$ than with respect to the full N-body problem. This problem was the original motivation for the work,[2] where we modified the construction precisely such as to make the approximations completely N-independent and accessible to computations. Eventually, this also led to Ref. 1, which was partially intended as a rigorous motivation of the assumptions on the initial data in Ref. 2.

IV. OPEN PROBLEMS

There are several open questions related to the results presented here. First, it would be interesting to generalize the dynamical analysis (Theorem 2) to the class of unbounded interaction potentials considered in Sec. II E 1 for the static problem, which, in particular, includes the Coulomb potential.

In addition, one can attempt to push the analysis to singular interactions of the type

$$v_{N,\beta}(x) = N^{-1+d\beta} v(N^\beta x), \qquad \beta \in [0,1],$$

for some bounded and compactly supported interaction potential v, where β is a scaling parameter interpolating from the Hartree ($\beta = 0$) to the Gross–Pitaevskii regime ($\beta = 1$). We expect the analysis to become harder with increasing β, mainly because of the emergence of an N-dependent short-scale correlation structure. Whereas new ideas are needed to cope with the extremely singular Gross–Pitaevskii regime, we expect our analysis to extend to a certain range of positive β.

Another interesting open problem is proving Borel summability of the asymptotic series in Theorems 1 and 2, at least for bounded interaction potentials. This property was established in Ref. 18 for the corresponding dynamical problem on Fock space described in

Sec. III E; hence, we conjecture that it should hold true also in the N-body setting, at least for bounded interaction potentials. As our current estimates of the growth of the error $C(a)$ in the parameter a are insufficient, new ideas are needed to improve this.

Finally, we expect our asymptotic expansions to be useful in answering various open problems related to the mean-field Bose gas. For instance, one should be able to derive effective interactions between the quasi-particles as discussed in Ref. 22 and to prove corrections to the central limit theorem obtained in Ref. 23.

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AUTHOR DECLARATIONS

Conflict of Interest

The author has no conflicts to disclose.

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

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