Upper bound for the grand canonical free energy of the Bose gas in the Gross–Pitaevskii limit

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June 21, 2023

We consider a homogeneous Bose gas in the Gross–Pitaevskii limit at temperatures that are comparable to the critical temperature for Bose–Einstein condensation in the ideal gas. Our main result is an upper bound for the grand canonical free energy in terms of two new contributions: (a) the free energy of the interacting condensate is given in terms of an effective theory describing its particle number fluctuations, (b) the free energy of the thermally excited particles equals that of a temperature-dependent Bogoliubov Hamiltonian.

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1. Introduction and main results

1.1. Background and summary

The dilute Bose gas, that is, a bosonic system with rare but strong collisions, is one of the most fundamental and interesting models in quantum statistical mechanics. Its prominence is mostly due to the occurrence of the Bose–Einstein condensation (BEC) phase transition and its numerous phenomenological consequences. Triggered by the experimental realization of BEC in ultra cold alkali gases in 1995, see [4, 23], and by the subsequent experimental progress, in the past two decades there have been numerous mathematical investigations of dilute Bose gases in different parameter regimes.

The most relevant parameter regime for the description of modern experiments with cold quantum gases is the Gross–Pitaevskii (GP) limit. Here the scattering length of the interaction between the particles is scaled with the particle number N in such a way that the interaction energy, in the limit $N \to \infty$, is of the same order of magnitude as the spectral gap in the trap. It has been shown in [43] that the ground state energy per particle can, in this limit, be approximated by the minimum of the GP energy functional. Moreover, approximate ground states of a trapped Bose gases display BEC and superfluidity, see [39, 41]. The derivation of the GP energy functional has later been extended in [40, 56] to the case of rotating gases, see also [49]. In such a system, the one-particle density matrices of approximate ground states can be shown to converge to a convex combination of projections onto the minimizers of the GP energy functional.

As predicted by Bogoliubov in 1947 in [14], the subleading correction to the ground state energy of a dilute Bose gas is given by the ground state energy of a certain quadratic Hamiltonian (called Bogoliubov Hamiltonian). Recently, this claim could be proved in the GP limit for a homogeneous Bose gas in [10, 12], for a homogeneous Bose gas with a slightly more singular interaction (Thomas-Fermi limit) in [2, 15], and for a trapped Bose gas in [17, 18, 48, 50]. The two-dimensional case has been investigated in [20, 21]. In all these works it was also possible to compute the low-lying eigenvalues of the Hamiltonian as well as the corresponding eigenfunctions. Simplified approaches in the homogeneous case have been provided in [34, 35], and a second order upper bound for a system with hard core interactions was proved in [5]. A Bose gas in a box with Neumann boundary conditions has been studied in [13].

Low energy eigenstates provide an accurate description of a Bose gas at zero temperature. However, the understanding of the model at positive temperature is essential for the full description of experiments and crucial for the mathematical understanding of the BEC phase transition. In this case one is interested in the free energy and the Gibbs state, which are natural equivalents of the ground state energy and the corresponding eigenfunction. A trapped Bose gas in a combination of a thermodynamic limit in the trap and a GP limit was studied in [26]. There it could be shown that the difference between the free energy of the system and that of the ideal gas is approximately given by the minimum of the GP energy functional. Moreover, the one-particle density matrix of approximate minimizers of the free energy are, to leading order, given by the one of the ideal gas, where the condensate wave function has been replaced by the minimizer of the GP energy functional. This, in particular, establishes the existence of a BEC phase transition in the system. Comparable results have been obtained also for a homogeneous Bose gas, see [25].

Consider an approximate ground state of a trapped Bose gas. Its dynamics after the trapping potential has been switched off can, in the GP limit, be described by the time-dependent GP equation, see [7, 16, 28, 29, 36, 53]. The dynamics of approximate positive temperature states has so far been studied only for mean field (high density) systems. More information about the derivation of effective evolution equations for bosonic many-particle systems can be found in the reviews [8, 51].

The GP limit is appropriate to describe experiments with $10^2 - 10^6$ alkali atoms. In contrast, truly macroscopic samples with particle numbers of the order of the Avogadro constant $N_A \approx 6.022 \times 10^{23}$ are well-described by the thermodynamic limit followed by a dilute (i.e., low density) limit. The asymptotic behavior of the specific energy in this setting has been obtained in [27, 45]. Results in two and one space dimensions can be found in [46] and [3], respectively. Also the next-to-leading order correction (Lee–Huang–Yang (LHY) term) predicted in [37] could recently be established, see [6, 60] (upper bound), [31, 32] (lower bound), and [30] (comparable result in two space dimensions). A two-term expansion for the free energy of the three-dimensional system has been proved in [61] (upper bound) and [58] (lower bound), and for the two-dimensional system in [47] (upper bound) and [24] (lower bound). In the latter case the result depends on the critical temperature of the Berezinskii—Kosterlitz—Thouless critical temperature for superfluidity. Finally, a LHY type lower bound for the free energy at suitably low temperatures, where the contribution of the excitation spectrum and the LHY correction are of the same order, has been proved in [33]. For a more extensive list of references concerning static properties of Bose gases we refer to [42, 54].

In the present article we consider a homogeneous Bose gas in the GP limit at temperatures of the order of the critical temperature for BEC. Our main result is an upper bound for the grand canonical free energy in terms of two new contributions. The first is the free energy of the particle number fluctuations of the interacting condensate and is described by a suitable effective theory. The second new contribution is related to the free energy of thermal excitations over the condensate. For temperatures of the order of the critical temperature, the number of excited particles may be of the same order as the number of particles in the condensate, and Bogoliubov modes need to be described in terms of a *temperature-dependent Bogoliubov Hamiltonian*. To obtain our upper bound, we construct a trial state as follows: particles in the condensate are described by a convex combination of coherent states, which allows us to increasing their entropy. The excitations are described by a Gibbs state of free bosons with *Bogoliubov dispersion relation*. The resulting state is a convex combination of quasi-free states, which we further transform to include two-body correlations. To do this we employ a suitable second quantized quartic operator. When computing the energy of our trial state, this operator allows us to renormalize the interaction potential and to show that the result only depends on the scattering length.

1.2. Notation

For two functions a and b of the particle number and other parameters of the system, we use the notation $a \lesssim b$ to say that there exists a constant $C > 0$ independent of the parameters such that $a \leq Cb$. If we want to highlight that C depends on a parameter k we use the symbol $\lesssim_k$. If $a \lesssim b$ and $b \lesssim a$ we write $a \sim b$ and $a \simeq b$ means that a and b are equal to leading order in the limit considered. By $C, c > 0$ we denote generic constants, whose values may change from line to line. The Fourier coefficients of a periodic function $f : [0, L]^3 \to \mathbb{C}$ are denoted by $\hat{f}(p) = \int_{[0,L]^3} e^{-\mathrm{i}px} f(x)\, \mathrm{d}x$, and for two Fourier coefficients $\hat{f}, \hat{g}$ we define their convolution as

$$\hat{f} * \hat{g}(p) = L^{-3} \sum_{p \in (2\pi/L)\mathbb{Z}^3} \hat{f}(p-q)\hat{g}(q). \tag{1.1}$$

This, in particular, implies $\widehat{fg}(p) = \hat{f} * \hat{g}(p)$.

1.3. Fock space and Hamiltonian

We consider a system of bosons confined to a three dimensional flat torus Λ with side length L. In what follows, we could set $L = 1$ but we prefer to keep a length scale to explicitly display units in formulas. The one-particle Hilbert space of the system is given by $L^2(\Lambda, \mathrm{d}x)$, with $\mathrm{d}x$ denoting Lebesgue measure. We are interested in the grand canonical ensemble, that is, in a system with a fluctuating particle number. The Hilbert space of the entire system is therefore given by the bosonic Fock space

$$\mathscr{F}(L^2(\Lambda, \mathrm{d}x)) = \bigoplus_{n=0}^{\infty} L^2_{\mathrm{sym}}(\Lambda^n, \mathrm{d}x) \tag{1.2}$$

over $L^2(\Lambda, \mathrm{d}x)$. Here $L^2_{\mathrm{sym}}(\Lambda^n, \mathrm{d}x)$ denotes the closed linear subspace of $L^2(\Lambda^n, \mathrm{d}x)$ consisting of those functions $\Psi(x_1, ..., x_n)$ that are invariant under any permutation of the coordinates $x_1, ..., x_n \in \Lambda$. As usual, we define $L^2_{\mathrm{sym}}(\Lambda^0, \mathrm{d}x) = \mathbb{C}$.

On the n-particle Hilbert space $L^2_{\mathrm{sym}}(\Lambda^n, \mathrm{d}x)$ with $n \geq 1$ we define the Hamiltonian

$$\mathcal{H}_N^{(n)} = \sum_{i=1}^{n} -\Delta_i + \sum_{1 \leq i < j \leq n} v_N(d(x_i, x_j)), \tag{1.3}$$

where Δ denotes the Laplacian on the torus Λ and $d(x, y)$ is the distance between two points $x, y \in \Lambda$. In the realization of Λ as the set $[0, L]^3$, Δ is the usual Laplacian with periodic boundary conditions and $d(x, y) = \min_{k \in \mathbb{Z}^3} |x - y - kL|$. We also define $\mathcal{H}_N^{(0)} = 0$. The interaction potential is of the form

$$v_N(d(x, y)) = N^2 v(N d(x, y)) \tag{1.4}$$

with a measurable, compactly supported function $v : [0, \infty) \to [0, \infty]$ and a parameter $N > 0$. We will later choose N as the expected number of particles in the system. Our assumptions on v guarantee that it has a finite scattering length $\mathfrak{a} \geq 0$. The scattering length is a combined measure for the range and the strength of an interaction potential. For its definition we refer to [42, Appendix C] and Appendix A. A simple scaling argument shows that the scattering length of v_N is given by $\mathfrak{a}_N = \mathfrak{a}/N$. Finally, the Hamiltonian $\mathcal{H}_N$ acting on $\mathscr{F}$ is defined by

$$\mathcal{H}_N = \bigoplus_{n=0}^{\infty} \mathcal{H}_N^{(n)}. \tag{1.5}$$

1.4. Grand canonical free energy, Gibbs state and Gibbs variational principle

We are interested in a gas of bosons in the grand canonical ensemble. The usual thermodynamic variables used to describe such a system are the inverse temperature, the chemical potential and the volume of the container. The chemical potential can later be chosen to obtain a desired particle number. In this article we replace the chemical potential in the above list of variables by the expected number of particles, which yields an equivalent description of the system. This motivates the following definitions.

The set of states on the bosonic Fock space $\mathscr{F}(L^2(\Lambda, \mathrm{d}x))$ with an expected number of $N \geq 0$ particles is defined by

$$\mathcal{S}_N = \{\Gamma \in \mathcal{B}(\mathscr{F}) \mid \Gamma \geq 0, \operatorname{Tr}\Gamma = 1, \operatorname{Tr}[\mathcal{N}\Gamma] = N\}, \tag{1.6}$$

where

$$\mathcal{N} = \bigoplus_{n=0}^{\infty} n \tag{1.7}$$

denotes the number operator on $\mathscr{F}$. For a state $\Gamma \in \mathcal{S}_N$, the Gibbs free energy functional reads

$$\mathcal{F}(\Gamma) = \operatorname{Tr}[\mathcal{H}_N \Gamma] - \frac{1}{\beta} S(\Gamma) \quad \text{with the von-Neumann entropy} \quad S(\Gamma) = -\operatorname{Tr}[\Gamma \ln(\Gamma)] \tag{1.8}$$

and the inverse temperature $\beta > 0$. The grand canonical free energy of the system is defined as the minimum of $\mathcal{F}$ in the set $\mathcal{S}_N$:

$$F(\beta, N, L) = \min_{\Gamma \in \mathcal{S}_N} \mathcal{F}(\Gamma) = -\frac{1}{\beta} \ln\left(\mathrm{Tr}[\exp(-\beta(\mathcal{H}_N - \mu\mathcal{N}))]\right) + \mu N. \tag{1.9}$$

Here the chemical potential μ is chosen such that the unique minimizer

$$G = \frac{\exp(-\beta(\mathcal{H}_N - \mu\mathcal{N}))}{\mathrm{Tr}[\exp(-\beta(\mathcal{H}_N - \mu\mathcal{N}))]} \tag{1.10}$$

of $\mathcal{F}$ satisfies $\mathrm{Tr}[\mathcal{N}G] = N$. The state G is called the (grand canonical) Gibbs state.

1.5. The ideal Bose gas on the torus

The bound that we prove for the free energy $F(\beta, N, L)$ in (1.9) depends on several quantities related to the ideal Bose gas on the torus. In this section we recall their definition and briefly discuss their behavior as a function of the inverse temperature β.

The chemical potential $\mu_0(\beta, N, L) < 0$ of the ideal gas is defined as the unique solution to the equation

$$N = \sum_{p \in \Lambda^*} \frac{1}{\exp(\beta(p^2 - \mu_0(\beta, N, L))) - 1}, \tag{1.11}$$

where $\Lambda^* = (2\pi/L)\mathbb{Z}^3$. The expected number of particles with momentum $p = 0$ and their density read

$$N_0(\beta, N, L) = (\exp(-\beta\mu_0) - 1)^{-1} \quad \text{and} \quad \varrho_0(\beta, N, L) = N_0(\beta, N, L)/L^3, \tag{1.12}$$

respectively. The asymptotic behavior of N_0 in the limit $N \to \infty$ is given by

$$\frac{N_0(\beta, N, L)}{N} \simeq \left[1 - \frac{\beta_c}{\beta}\right]_+ \quad \text{with} \quad \beta_c = \frac{1}{4\pi}\left(\frac{N}{L^3\zeta(3/2)}\right)^{-2/3}. \tag{1.13}$$

We note that β in (1.13) usually depends on N. By ζ we denote the Riemann zeta function and $[x]_+ = \max\{0, x\}$. The above formula implies that the ideal Bose gas displays a BEC phase transition: If $\beta = \kappa\beta_c$ with $\kappa \in (1, \infty)$ then $N_0 \simeq N[1 - 1/\kappa]$ and $|\mu_0| \sim L^{-2}N^{-1/3}$. In contrast, for $\beta = \kappa\beta_c$ with $\kappa \in (0, 1)$ we have $N_0 \sim 1$ and $|\mu_0| \sim L^{-2}N^{2/3}$. Finally, the grand canonical free energy of the ideal gas is given by $F_0 = F_0^{\mathrm{BEC}} + F_0^{+}$. Here

$$F_0^{\mathrm{BEC}}(\beta, N, L) = \frac{1}{\beta} \ln\left(1 - \exp(\beta\mu_0)\right) + \mu_0 N_0 \tag{1.14}$$

denotes the free energy of the condensate and

$$F_0^{+}(\beta, N, L) = \frac{1}{\beta} \sum_{p \in \Lambda_+^*} \ln\left(1 - \exp\left(-\beta(p^2 - \mu_0)\right)\right) + \mu_0(N - N_0) \tag{1.15}$$

that of the non-condensed particles.

1.6. Main results

Our main result is the following upper bound for the free energy of the homogeneous Bose gas in the GP limit.

Theorem 1.1. *Assume that the function $v : [0,\infty) \to [0,\infty]$ is nonnegative, compactly supported, and satisfies $v(|\cdot|) \in L^3(\Lambda, \mathrm{d}x)$. By $\varrho = N/L^3$ we denote the particle density. In the combined limit $N \to \infty$, $\beta = \kappa\beta_c$ with $\kappa \in (0,\infty)$ and β_c in (1.13), the free energy in (1.9) satisfies the upper bound*

$$F(\beta,N,L) \leq F_0^+(\beta,N,L) + 8\pi\mathfrak{a}_N L^3\varrho^2 + \min\{F^{\mathrm{BEC}} - 8\pi\mathfrak{a}_N L^3\varrho_0^2, F_0^{\mathrm{BEC}}\} \\ - \frac{1}{2\beta}\sum_{p\in\Lambda_+^*}\left[\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2}\right)\right] + O(L^{-2}N^{7/12}), \tag{1.16}$$

with ϱ_0 in (1.12), F_0^{BEC} in (1.14), F_0^+ in (1.15), and

$$F^{\mathrm{BEC}}(\beta,N_0,L,\mathfrak{a}_N) = -\frac{1}{\beta}\ln\left(\int_{\mathbb{C}}\exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \mu|z|^2\right)\right)\mathrm{d}z\right) + \mu N_0(\beta,N,L). \tag{1.17}$$

Here $\mathrm{d}z = \mathrm{d}x\,\mathrm{d}y/\pi$, where x and y denote the real and imaginary part of the complex number z, respectively. The chemical potential μ in (1.17) is chosen such that the Gibbs distribution

$$g(z) = \frac{\exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \mu|z|^2\right)\right)}{\int_{\mathbb{C}}\exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \mu|z|^2\right)\right)\mathrm{d}z} \quad \text{satisfies} \quad \int_{\mathbb{C}}|z|^2 g(z)\,\mathrm{d}z = N_0(\beta,N,L). \tag{1.18}$$

The terms on the r.h.s. of (1.16) are listed in descending order concerning their order of magnitude in the limit $N \to \infty$. The free energy of the non-condensed particles satisfies $F_0^+ \sim L^{-2}N^{5/3}$. The second term is a density-density interaction of the order $L^{-2}N$. As we will see with Proposition 1.2 below, the energy of the interacting condensate (the third term), contributes on two orders of magnitude (if $\kappa > 1$): $L^{-2}N$ and $L^{-2}N^{2/3}\ln(N)$. The term in the second line is a correction to the free energy of the non-condensed particles coming from Bogoliubov theory, and is of the order $L^{-2}N^{2/3}$.

The following proposition provides us with a simplified expression for F^{BEC} above and below the critical point. This, in particular, allows us to compute the minimum on the r.h.s. of (1.16).

Proposition 1.2. *The following statements hold for given $\varepsilon > 0$ in the limit $N \to \infty$:*

(a) Assume that $N_0 \gtrsim N^{5/6+\varepsilon}$. There exists a constant $c > 0$ such that

$$F^{\mathrm{BEC}}(\beta,N_0,L,\mathfrak{a}_N) = 4\pi\mathfrak{a}_N L^{-3}N_0^2 + \frac{\ln\left(4\beta\mathfrak{a}_N/L^3\right)}{2\beta} + O\left(L^{-2}\exp\left(-cN^{\varepsilon}\right)\right). \tag{1.19}$$

(b) Assume that $N_0 \lesssim N^{5/6-\varepsilon}$. Then

$$F^{\mathrm{BEC}}(\beta,N_0,L,\mathfrak{a}_N) = -\frac{1}{\beta}\ln(N_0) - \frac{1}{\beta} + O\left(L^{-2}N^{2/3-2\varepsilon}\right) \tag{1.20}$$

holds. In particular, $F^{\mathrm{BEC}}(\beta,N_0,L,\mathfrak{a}_N)$ is independent of $\mathfrak{a}_N$ at the given level of accuracy.

The interpretation of Proposition 1.2 is as follows: if the number of particles in the BEC is sufficiently large, we see a contribution of the order $L^{-2}N^{2/3}\ln(N)$ in addition to the density-density interaction $4\pi\mathfrak{a}_N L^{-3}N_0^2$. This new contribution (the second term on the r.h.s. of (1.19)) is a consequence of the particle number fluctuations in the BEC and will be discussed in more detail in Remark 1.4.(b) below. In contrast, if the expected particle number inside the BEC satisfies $1 \ll N_0 \leq N^{5/6-\varepsilon}$ its free energy equals that of an ideal gas to leading order. The appearance of the exponent $5/6$ is explained by the fact that $4\pi\mathfrak{a}_N L^{-3}N_0^2 \sim L^{-2}N^{2/3}$ if $N_0 \sim N^{5/6}$. This should be compared to $1/\beta$ times the classical entropy of g (for a definition see (1.25) below), which, for $N^{\varepsilon} \leq N_0 \leq N^{5/6}$ with $\varepsilon > 0$, is always of the order $\ln(N)/\beta \sim L^{-2}N^{2/3}\ln(N)$. That is, in the parameter region

$N^{5/6-\varepsilon} \lesssim N_0 \lesssim N^{5/6+\varepsilon}$ the effective theory of the condensate transitions from a regime where the interaction is relevant to a regime where it is not. For those values of N_0 the free energy F^{BEC} does not have a form that is as simple as that in (1.19) or (1.20).

Proposition 1.2 allows us to bring our main result into a form that is better suited for a comparison to the existing literature, as stated in the following Corollary.

Corollary 1.3. *Assume that the function $v : [0,\infty) \to [0,\infty]$ is nonnegative, compactly supported, and satisfies $v(|\cdot|) \in L^3(\Lambda, \mathrm{d}x)$. By $\varrho = N/L^3$ we denote the particle density. We consider the combined limit $N \to \infty$, $\beta = \kappa\beta_c$ with $\kappa \in (0,\infty)$ and β_c in (1.13). If $\kappa \in (1,\infty)$ the free energy in (1.9) satisfies the upper bound*

$$\begin{aligned} F(\beta,N,L) \leq & F_0^+(\beta,N,L) + 4\pi\mathfrak{a}_N L^3 \left(2\varrho^2 - \varrho_0^2(\beta,N,L)\right) + \frac{\ln\left(4\beta\mathfrak{a}_N/L^3\right)}{2\beta} \\ & - \frac{1}{2\beta}\sum_{p\in\Lambda_+^*}\left[\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2}\right)\right] + O(L^{-2}N^{7/12}) \end{aligned} \tag{1.21}$$

and if $\kappa \in (0,1)$ we have

$$F(\beta,N,L) \leq F_0(\beta,N,L) + 8\pi\mathfrak{a}_N L^3\varrho^2 + O(L^{-2}N^{1/2}) \tag{1.22}$$

with F_0 defined above (1.14).

If $\kappa \in (1,\infty)$ the minimum in (1.16) is attained by the first term and one obtains (1.21). In contrast, for $\kappa \in (0,1)$ it equals the second term, which leads to (1.22). At the critical point ($\kappa = 1$) the minimum is needed. We have the following remarks concerning the above statements.

Remark 1.4. (a) The first two terms on the r.h.s. of (1.21) and (1.22) already appeared in an asymptotic expansion of the canonical free energy in the GP limit in [25] (with a remainder of the order $o(L^{-2}N)$). To be precise, the result in (1.21) has been stated with F_0^+ replaced by the canonical free energy F_0^{c} of the ideal gas. From [25, Lemma A1] we, however, know that F_0^{c} and F_0^+ agree up to a remainder of the order $L^{-2}N^{2/3}\ln(N)$. It is to be expected that the result in [25] also holds if the grand canonical ensemble is considered. That is, the two ensembles are expected to be equivalent if one allows for remainders of the order $o(L^{-2}N)$. We highlight that the first two terms on the r.h.s. of (1.21) had for the first time been justified in the thermodynamic limit, see [61] (upper bound) and [58] (lower bound). The inclusion of the remaining two (negative) terms in the upper bound for the free energy in (1.21) is therefore our main new contribution.

(b) The third term on the r.h.s. of (1.21) is related to the particle number fluctuations in the BEC. Let us explain this in some more detail: it is well known that a c-number substitution for one momentum mode in the spirit of [25, 44] (method of coherent states) introduces only a small correction to the free energy. Motivated by this, we use a trial state of the form

$$\Gamma_0 = \int_{\mathbb{C}} |z\rangle\langle z|\, p(z)\,\mathrm{d}z, \qquad \text{where} \qquad |z\rangle = \exp(za_0^* - \overline{z}a_0)|\mathrm{vac}\rangle \tag{1.23}$$

to describe the BEC. Here a_0^* and a_0 denote the usual creation and annihilation operators of a particle in the $p = 0$ mode and $|\mathrm{vac}\rangle$ is the related vacuum vector. Moreover, $p(z)$ is a probability distribution on $\mathbb{C}$ w.r.t. the measure $\mathrm{d}z$ defined below (1.17). Let us assume that the interaction energy of the BEC is described by the effective Hamiltonian $4\pi\mathfrak{a}_N L^{-3} a_0^* a_0^* a_0 a_0$. The free energy of Γ_0 is then given by

$$\mathcal{F}^{\mathrm{BEC}}(\Gamma_0) = 4\pi\mathfrak{a}_N L^{-3}\int_{\mathbb{C}} |z|^4 p(z)\,\mathrm{d}z - \frac{1}{\beta}S(\Gamma_0). \tag{1.24}$$

From the the Berezin–Lieb inequality, see e.g. [9, 38], we know that the last term on the r.h.s. is bounded from above by $-1/\beta$ times

$$S(p) = -\int_{\mathbb{C}} p(z) \ln(p(z)) \, dz. \tag{1.25}$$

When we minimize $\mathcal{F}^{\text{BEC}}(\Gamma_0)$ with $S(\Gamma_0)$ replaced by $S(p)$ under the constraint $\int |z|^2 p(z) \, dz = N_0$ over all probability distributions p, we obtain F^{BEC} in (1.17). The unique minimizer is the Gibbs distribution g in (1.18). With the above considerations, Proposition 1.2.(a), and $\int_{\mathbb{C}} |z|^2 g(z) \, dz = N_0$ we conclude that

$$4\pi \mathfrak{a}_N L^{-3} \left(\int_{\mathbb{C}} |z|^4 g(z) \, dz - \left(\int_{\mathbb{C}} |z|^2 g(z) \, dz \right)^2 \right) - \frac{1}{\beta} S(g) = \frac{\ln\left(16\beta\mathfrak{a}_N/L^3\right)}{2\beta} + O\left(L^{-2} \exp\left(-cN^{\varepsilon/2}\right)\right) \tag{1.26}$$

provided that $N_0 \geq N^{5/6+\varepsilon}$ holds for some fixed $\varepsilon > 0$. That is, the term on the r.h.s. of the above equation indeed describes the free energy related to the particle number fluctuations in the BEC. It is interesting to note that this contribution vanishes in the thermodynamic limit because it is bounded from above by a constant times $\ln(N)/\beta$.

(c) The Gibbs distribution g in (1.18) satisfies

$$\text{Var}_g(|z|^2) = \int_{\mathbb{C}} |z|^4 g(z) \, dz - \left(\int_{\mathbb{C}} |z|^2 g(z) \, dz \right)^2 \sim N^{5/3} \tag{1.27}$$

for ($\kappa > 1$), which should be compared to the grand canonical ideal Bose gas. Here the same quantity is of the order N^2. This decrease of the number fluctuations in the BEC is a well-known effect caused by the repulsive interaction between the particles. Motivated by the recent experimental realization of a system with grand canonical number statistics, see [55], a discrete version of g in (1.18) has recently been used in [59] to compute the particle number fluctuations in an interacting grand canonical trapped BEC. To rigorously justify the computations in [59], it is necessary to show that $g(z)$ approximates $\text{Tr}[|z\rangle\langle z| G]$ with the interacting Gibbs state G in (1.10). This is a very interesting mathematical problem, whose solution is beyond the scope of the present investigation.

(d) The term in the second line of (1.21) is a correction to the free energy of the non-condensed particles coming from Bogoliubov theory. It can be motivated by the following heuristic computation: We write the Hamiltonian $\mathcal{H}_N$ in (1.5) in terms of creation and annihilation operators a_p and a_p^* of a particle with momentum $p \in \Lambda^*$. Next we replace a_0 and a_0^* by $\sqrt{N_0}$, and $\hat{v}(p)$ by $4\pi\mathfrak{a}_N L^{-3}$. When we additionally neglect cubic and quartic terms in a_p and a_p^*, we obtain the Bogoliubov Hamiltonian

$$\mathcal{H}^{\text{Bog}} = \sum_{p \in \Lambda_+^*} p^2 a_p^* a_p + 4\pi\mathfrak{a}_N \varrho_0(\beta, N, L) \sum_{p \in \Lambda_+^*} \left(2a_p^* a_p + a_p^* a_{-p}^* + a_p a_{-p} \right). \tag{1.28}$$

A careful analysis shows that the grand potential $\Phi^{\text{Bog}}(\beta, \mu_0, L)$ associated to $\mathcal{H}^{\text{Bog}}$ with μ_0 in (1.11) satisfies (compare to Lemma B.1 in Appendix B)

$$\begin{aligned} \Phi^{\text{Bog}}(\beta, \mu_0, L) =& \frac{1}{\beta} \sum_{p \in \Lambda_+^*} \ln\left(1 - \exp\left(\beta |p^2 - \mu_0| \sqrt{p^2 - \mu_0 + 16\pi\mathfrak{a}_N \varrho_0}\right)\right) \\ =& \frac{1}{\beta} \sum_{p \in \Lambda_+^*} \ln\left(1 - \exp\left(-\beta(p^2 - \mu_0)\right)\right) + 8\pi\mathfrak{a}_N L^3 (\varrho - \varrho_0)\varrho_0 \\ & - \frac{1}{2\beta} \sum_{p \in \Lambda_+^*} \left[\frac{16\pi\mathfrak{a}_N \varrho_0(\beta, N, L)}{p^2} - \ln\left(1 + \frac{16\pi\mathfrak{a}_N \varrho_0(\beta, N, L)}{p^2}\right) \right] + o(L^{-2} N^{2/3}). \end{aligned} \tag{1.29}$$

The first term on the r.h.s. contributes to F_0^+, the second term is part of the density-density interaction energy, and the third term is the novel contribution in the second line of (1.21).

(e) In [10] it has been shown that eigenvalues E of $\mathcal{H}_N^{(N)}$ in (1.3) that satisfy $E \ll L^{-2}N^{1/8}$ are, to leading order, as $N \to \infty$, approximated by those of a Bogoliubov Hamiltonian. If we compare this energy scale to our temperature $1/\beta \sim 1/\beta_c \sim L^{-2}N^{2/3}$, which is a measure for the *energy per particle* in our system, we see that the result in [10] is far from being sufficient to draw conclusions about the free energy.

(f) It is interesting to note that if one replaces $\mathfrak{a}_N$ by $\mathfrak{a}$ and takes the thermodynamic limit ($N, L \to \infty$ with $\varrho = N/L^3$ fixed) of the last term in (1.29) divided by L^3, one obtains

$$-\frac{1}{2\beta(2\pi)^3}\int_{\mathbb{R}^3}\left[\frac{16\pi\mathfrak{a}\varrho_0}{p^2} - \ln\left(1 + \frac{16\pi\mathfrak{a}\varrho_0}{p^2}\right)\right]\mathrm{d}p = -\frac{16\sqrt{\pi}}{3\beta}(\mathfrak{a}\varrho_0)^{3/2}. \tag{1.30}$$

The r.h.s. has been conjectured to appear in the asymptotic expansion of the specific free energy in the dilute limit, see [52, Theorem 11]. There it is shown that minimizing the free energy functional (1.8) over the class of quasi-free states leads to (1.30) with the scattering length replaced by its first Born approximation.

(g) The minimum in the third term on the r.h.s. of (1.16) is needed because F^{BEC} fails to describe the free energy of the BEC correctly if $N_0 \sim 1$ ($\Leftrightarrow \kappa < 1$). This is related to the fact that we describe the discrete random variable associated to the operator $a_0^* a_0$ by one that is continuous.

(h) Theorem 1.1 is stated and proved for fixed $\kappa \in (0, \infty)$. Our proof can, however, easily be extended to cover the case when κ depends on N provided $\kappa \gtrsim 1$ holds.

(i) We expect the upper bound in Theorem 1.1 to be accurate up to a remainder of the order $o(L^{-2}N^{2/3})$. That is, we expect it to be possible to prove a matching lower bound.

(j) In case of the canonical ensemble we expect that $F_0^+ + F^{\mathrm{BEC}}$ needs to replaced by $F_0^{\mathrm{c}} + 4\pi\mathfrak{a}_N\varrho_0^2$, where F_0^{c} denotes the free energy of the canonical ideal gas. This is a consequence of the fact the variance of the number of condensed particles in the canonical ideal gas lives, for $\beta = \kappa\beta_c$ with $\kappa > 1$, on the scale $N^{4/3}$. This needs to be compared to (1.27) and (1.26). For a thorough analysis of condensate fluctuations in the canonical ideal gas we refer to [22].

1.7. Organization of the article

We prove Theorem 1.1 with a trial state argument. In Section 2 we define our trial state and establish some of its properties that are needed for proving an upper bound for its free energy. In Section 3, which is the core of our analysis, we provide an upper bound for the energy of our trial state, and Section 4 is devoted to an estimate for its entropy. Finally, in Section 5 we use these results to give the proof of Theorem 1.1. To not dilute the main line of the argument, we deferred some technical parts of our proof to an Appendix. In Appedix A we collect known properties of the solution to the scattering equation in a ball with Neumann boundary conditions. Appendix B contains the proof of an expansion of the free energy related to a Bogoliubov Hamiltonian in the spirit of (1.29). Finally, in Appendix C we prove Proposition 1.2 as well as some lemmas concerning F^{BEC} in (1.17) and g in (1.18).

2. The trial state

In this section we define our trial state and collect some of its properties.

2.1. Definition of the trial state

We start our analysis with the definition of a trial state. To be able to distinguish between different parts of the system as e.g. the condensate, thermally excited particles, and the microscopic correlations between the particles induced by v_N, we start by introducing several subsets of the momentum space Λ^*. Let $\delta_\mathrm{B}, \delta_\mathrm{L}, \delta_\mathrm{H} > 0$ with $\delta_\mathrm{B} < 1/3$ and $\delta_\mathrm{L} + \delta_\mathrm{H} < 2/3$ and define

$$\begin{aligned}
P_\mathrm{L} &:= \left\{ p \in \Lambda^* \mid |p| \leq N^{1/3+\delta_\mathrm{L}}/L \right\}, \\
P_\mathrm{B} &:= \left\{ p \in \Lambda^* \mid 0 < |p| \leq N^{\delta_\mathrm{B}}/L \right\}, \\
P_\mathrm{I} &:= \left\{ p \in \Lambda^* \mid N^{\delta_\mathrm{B}}/L < |p| \leq N^{1/3+\delta_\mathrm{L}}/L \right\}, \\
P_\mathrm{H} &:= \left\{ p \in \Lambda^* \mid |p| \geq N^{1-\delta_\mathrm{H}}/L \right\}.
\end{aligned} \tag{2.1}$$

Our assumptions on the parameters assure that $P_\mathrm{B} \subset P_\mathrm{L}$ and $P_\mathrm{L} \cap P_\mathrm{H} = \emptyset$. Later, all parameters defined above will be chosen independently of N. The meaning of our sets in (2.1)–(2.1) is the following: the set P_L is appropriate to describe the BEC and the thermally excited particles described by our trial state. To that end, it is sufficient to choose $\delta_\mathrm{L} > 0$ as small as we wish. For any $\delta_\mathrm{B} > 0$, the set P_B is large enough to describe the Bogoliubov excitations in the system. The part of the trial state with support in $\mathscr{F}(L^2(P_\mathrm{I}))$ will be chosen as the Gibbs state of an ideal gas. That is, for these modes Bogoliubov theory is not relevant. Finally, the microscopic correlations between the particles induced by the singular interaction v_N will be chosen to live in the set P_H.

It is convenient for us to introduce the following decomposition of the bosonic Fock space:

$$\mathscr{F}(L^2(\Lambda, \mathrm{d}x)) \cong \mathscr{F}_0 \otimes \mathscr{F}_\mathrm{B} \otimes \mathscr{F}_\mathrm{I} \otimes \mathscr{F}_>, \tag{2.2}$$

where $\mathscr{F}_0$ denotes the Fock space over the $p = 0$ mode, $\mathscr{F}_\mathrm{B}$ is the Fock space over $L^2(P_\mathrm{B})$, $\mathscr{F}_\mathrm{I}$ denotes the Fock space over $L^2(P_\mathrm{I})$, and $\mathscr{F}_>$ is the Fock space over all remaining momentum modes. Moreover, by $\cong$ we denote unitary equivalence. In the following we will, without explicitly mentioning it, use the same symbol for an operator acting on $\mathscr{F}$ and for its unitary image acting on $\mathscr{F}_0 \otimes \mathscr{F}_\mathrm{B} \otimes \mathscr{F}_\mathrm{I} \otimes \mathscr{F}_>$. By $a^*(g)$ and $a(g)$ we denote the usual creation and annihilation operators of a particle in the function $g \in L^2(\Lambda, \mathrm{d}x)$, which satisfy the canonical commutation relations

$$[a(g), a^*(h)] = \langle g, h \rangle, \quad [a(g), a(h)] = 0 = [a^*(g), a^*(h)]. \tag{2.3}$$

We also use the notation $a_p = a(\varphi_p)$ with the plane wave $L^{-3/2} e^{\mathrm{i}px}$. In this special case the first identity in (2.3) reads $[a_p, a_q^*] = \delta_{p,q}$.

We are now prepared to define our trial state and start by introducing the Bogoliubov Hamiltonian

$$\mathcal{H}^\mathrm{B} = \sum_{p \in P_\mathrm{B}} (p^2 - \mu_0) a_p^* a_p + \frac{\varrho_0(\beta, N, L)}{2} \sum_{p \in P_\mathrm{B}} \hat{v}_N * \hat{f}_N(p) \left[2a_p^* a_p + (z/|z|)^2 a_p^* a_{-p}^* + (\overline{z}/|z|)^2 a_p a_{-p} \right] \tag{2.4}$$

with μ_0 in (1.11), ϱ_0 in (1.12), and the Fourier coefficients $\hat{f}_N = \int_\Lambda e^{-\mathrm{i}px} v_N(x) \, \mathrm{d}x$ of the solution $f_N(x)$ to a version of the zero energy scattering equation that will be introduced more carefully below. We also recall our definition of the convolution in (1.1). By

$$G_\mathrm{B}(z) = \frac{\exp(-\beta \mathcal{H}^\mathrm{B})}{\mathrm{Tr}_{\mathscr{F}_\mathrm{B}}[\exp(-\beta \mathcal{H}^\mathrm{B})]} \tag{2.5}$$

we denote the Gibbs state related to $\mathcal{H}^\mathrm{B}$, which acts on $\mathscr{F}_\mathrm{B}$. We also introduce the Gibbs state of the ideal gas

$$G_\mathrm{free} = \frac{\exp(-\beta \, \mathrm{d}\Gamma(\mathbb{1}(-\mathrm{i}\nabla \in P_\mathrm{I})(-\Delta - \mu_0)))}{\mathrm{Tr}_{\mathscr{F}_\mathrm{I}} \exp(-\beta \, \mathrm{d}\Gamma(\mathbb{1}(-\mathrm{i}\nabla \in P_\mathrm{I})(-\Delta - \mu_0)))}, \tag{2.6}$$

acting on $\mathscr{F}_\mathrm{I}$. With these definitions at hand, we define the state Γ_0 without microscopic correlations between the particles by

$$\Gamma_0 = \int_\mathbb{C} |z\rangle\langle z| \otimes G_\mathrm{B}(z) \zeta(z) \, \mathrm{d}z \otimes G_\mathrm{free}. \tag{2.7}$$

Here $|z\rangle$ is the coherent state in (1.23). The probability distribution $\zeta(z)$ is given by

$$\zeta(z) = \frac{\exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \widetilde{\mu}|z|^2\right)\right)}{\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi\mathfrak{a}_N L^{-3}|z|^4 - \widetilde{\mu}|z|^2\right)\right) \mathrm{d}z} \tag{2.8}$$

i.e., it equals $g(z)$ in (1.18) except for the fact that the chemical potential $\widetilde{\mu}$ in the definition of ζ is chosen s.t. $\mathrm{Tr}[\mathcal{N}\Gamma_0] = N$ holds (see also (2.34) below). Since the chemical potential in the definition of $G_{\mathrm{B}}(z)$ is fixed this may be possible only if N is large enough. We define $\widetilde{N}_0$ by

$$\widetilde{N}_0 = \int_{\mathbb{C}} |z|^2 \zeta(z)\, \mathrm{d}z. \tag{2.9}$$

In Lemma 2.6 we show that $\widetilde{N}_0$ equals N_0 in (1.12) up to a correction of the order $L^2 N_0/(\beta N) \sim N^{2/3}$ if $N_0 \sim N$. In the computation of the free energy of our trial state we obtain the term $F^{\mathrm{BEC}}(\beta, \widetilde{N}_0, L, \mathfrak{a}_N)$. To replace this free energy by the same expression with $\widetilde{N}_0$ replaced by N_0, we use Lemma C.1 in Appendix C. It is important to note that the difference between these two free energies yields a contribution of the order $L^{-2}N_0^2/N$. More details concerning this issue can be found in Section 5 in the analysis following (5.16).

The definition of the condensate part and the part of our trial state related to the Bogoliubov modes $p \in P_{\mathrm{B}}$ have been motivated in Remark 1.4.(b) and (d), respectively. For higher momenta the Bogoliubov dispersion relation $\sqrt{p^2 - \mu_0}\sqrt{p^2 - \mu_0 + 16\pi\mathfrak{a}_N\varrho_0}$ resembles $p^2 - \mu_0$, to leading order. We find it therefore more convenient to describe the thermally excited particles with momenta in P_{I} by G_{free}. The Bogoliubov Hamiltonian in (2.4) depends on $z/|z|$ because the condensate is described by the coherent state $|z\rangle\langle z|$. The complex phase $z/|z|$ will cancel out in the computation of the energy but its inclusion here is crucial for certain terms not to vanish.

In the final step, we dress our trial state with a correlation structure that describes the microscopic correlations introduced by v_N. Let f_N denote the ground state solution to the Neumann problem

$$(-\Delta + v_N(x)/2) f_N(x) = \lambda_N f_N(x) \tag{2.10}$$

on the ball $B_\ell(0)$ with some fixed $0 < \ell < L/2$. We assume that f_N is normalized such that it equals 1 on $\partial B_\ell(0)$ and we interpret it as a function on Λ by extending it by 1 outside of $B_\ell(0)$. Eq (2.10) is a finite volume version of the zero energy scattering equation $\Delta f(x) = v(x) f(x)/2$ with boundary condition $\lim_{|x|\to\infty} f(x) = 1$ on $\mathbb{R}^3$. We also define

$$\eta_p = \hat{f}_N(p) - |\Lambda|\delta_{p,0}. \tag{2.11}$$

More information on the functions f_N and η_p can be found in Appendix A. With η_p at hand, we define the two-body operator

$$B = \frac{1}{2|\Lambda|} \sum_{p \in P_{\mathrm{H}},\, u,v \in P_{\mathrm{L}}} \eta_p\, a^*_{u+p} a^*_{v-p} a_u a_v \tag{2.12}$$

on $\mathscr{F}$. Except for the restriction of the momenta, it is a multiplication operator with the inverse Fourier transform of the function η_p. We apply the spectral theorem to write $\Gamma_0 = \sum_\alpha \lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|$ and define our trial state Γ by

$$\Gamma = \sum_{\alpha=1}^{\infty} \lambda_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|, \quad \text{where} \quad \phi_\alpha = \frac{(1+B)\psi_\alpha}{\|(1+B)\psi_\alpha\|}. \tag{2.13}$$

The general idea behind the way we introduce correlations is as follows: let us for the sake of simplicity consider an N-particle wave function ψ that we want to dress. A natural way to introduce correlations is to multiply ψ with a Jastrow factor $\prod_{i<j} f_N(x_i - x_j)$. When we write $f_N = 1 - w_N$ and expand the product in powers of w_N, we obtain $(1 - \sum_{i<j} w_N(x_i - x_j))\psi$ plus higher order contributions in w_N. Except for our

momentum cut-offs, these first two terms equal $(1+B)\psi$. Since higher order corrections in w_N are not necessary to obtain the correct energy in the GP limit, we omit these contributions. The restrictions of the momentum sums in the definition of B turn out to be mathematically convenient. Intuitively, $p \in P_{\mathrm{H}}$ and $u, v \in P_{\mathrm{L}}$ because η_p can be well approximated with momenta in P_{H} and $G_{\mathrm{B}}(z)$ and G_{free} can be well approximated with momenta in P_{L}. Correlation structures that are similar to the one introduced by B have been used at zero temperature in [10, 12]. A similar approach to describe correlations can be found in [60, 61]. In the remainder of this article, we prove an upper bound for the free energy of Γ that implies Theorem 1.1.

2.2. Preparatory lemmas

In this section we state and prove several lemmas that are needed for the computation of the free energy of Γ in (2.13). We present them here to not interrupt the main line of the argument in Section 3.

Properties of the state $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$

The first lemma provides us with a Bogoliubov transformation that diagonalizes the Bogoliubov Hamiltonian $\mathcal{H}^{\mathrm{B}}$ in (2.4). Before we state it, we introduce the following notation. For fixed $z \in \mathbb{C}$ and $p \in \Lambda^*$, we define the functions $\varphi_{p,z}(x) = (z/|z|)L^{-3/2}e^{\mathrm{i}px}$, which are planes waves with a z-dependent phase. By $a^*_{p,z} = a^*(\varphi_{p,z})$ and $a_{p,z} = a(\varphi_{p,z})$ we denotes the operators that create and annihilate a particle in the function $\varphi_{p,z}$, respectively. Since $\{\varphi_{p,z}\}_{p\in 2\pi\mathbb{Z}/L}$ is an orthonormal basis of $L^2(\Lambda, \mathrm{d}x)$ the operators $a^*_{p,z}$ and $a_{p,z}$ satisfy the canonical commutation relations in the form stated below (2.3). We also define the (unitary) Bogoliubov transformation $\mathcal{U}_z$ by its action on our z-dependent creation and annihilation operators in the following way ($p \in P_{\mathrm{B}}$):

$$\mathcal{U}_z^* a^*_{p,z} \mathcal{U}_z = u_p a^*_{p,z} + v_p a_{-p,z}, \qquad \mathcal{U}_z^* a_{p,z} \mathcal{U}_z = u_p a_{p,z} + v_p a^*_{-p,z}. \tag{2.14}$$

The z-independent coefficients u_p and v_p are defined by

$$\begin{aligned} u_p &= \frac{1}{2}\left(\frac{p^2-\mu_0}{p^2-\mu_0+2\hat{v}_N * \hat{f}_N(p)\varrho_0}\right)^{1/4} + \frac{1}{2}\left(\frac{p^2-\mu_0}{p^2-\mu_0+2\hat{v}_N * \hat{f}_N(p)\varrho_0}\right)^{-1/4} \quad \text{and} \\ v_p &= \frac{1}{2}\left(\frac{p^2-\mu_0}{p^2-\mu_0+2\hat{v}_N * \hat{f}_N(p)\varrho_0}\right)^{1/4} - \frac{1}{2}\left(\frac{p^2-\mu_0}{p^2-\mu_0+2\hat{v}_N * \hat{f}_N(p)\varrho_0}\right)^{-1/4} \end{aligned} \tag{2.15}$$

with μ_0 in (1.11) and ϱ_0 in (1.12), respectively. The function $\hat{v}_N * \hat{f}_N(p)$ may take negative values. However, we claim that there exists $\widetilde{N} \in \mathbb{N}$ such that it is nonnegative uniformly in $p \in P_{\mathrm{B}}$ provided $N \geq \widetilde{N}$. To prove this, we note that

$$\hat{v}_N * \hat{f}_N(p) \geq \hat{v}_N * \hat{f}_N(0) - |p| \int_0^1 |\nabla \hat{v}_N * \hat{f}_N(tp)| \,\mathrm{d}t \geq \hat{v}_N * \hat{f}_N(0) - N^{\delta_{\mathrm{B}}} L^{-1} \int_\Lambda v_N(x) f_N(x) |x| \,\mathrm{d}x. \tag{2.16}$$

By Lemma A.1 we know that $0 \leq f_N \leq 1$; we use this and $\int v_N(x) N|x| \,\mathrm{d}x / L = N^{-1} \| \,|\cdot| v \|_1$ to see that the last term on the r.h.s. is bounded by a constant times $LN^{\delta_{\mathrm{B}}-2}$. Since $0 < \delta_{\mathrm{B}} < 1/3$ by assumption, and $\hat{v}_N * \hat{f}_N(0) = N^{-1} \int v(x) f(x) \,\mathrm{d}x \gtrsim LN^{-1}$ by (A.3), the claim is proved. In particular, it assures that u_p and v_p are well defined. In the following we will always assume that $N \geq \widetilde{N}$, and hence $\hat{v}_N * \hat{f}_N(p) \geq 0$ for $p \in P_{\mathrm{B}}$.

We are now prepared to state our first lemma.

Lemma 2.1. *The Bogoliubov Hamiltonian $\mathcal{H}^{\mathrm{B}}$ in (2.4) satisfies*

$$\mathcal{U}_z^* \mathcal{H}^{\mathrm{B}} \mathcal{U}_z = E_0 + \sum_{p \in P_{\mathrm{B}}} \varepsilon(p) a^*_p a_p \tag{2.17}$$

with

$$\varepsilon(p) = \sqrt{p^2 - \mu_0}\sqrt{p^2 - \mu_0 + 2\hat{v}_N * \hat{f}_N(p)\varrho_0} \quad \text{and} \quad E_0 = -\frac{1}{2}\sum_{p\in P_{\mathrm{B}}}\left[p^2 - \mu_0 + \varrho_0\hat{v}_N * \hat{f}_N(p) - \varepsilon(p)\right]. \tag{2.18}$$

Proof. To see that the Bogoliubov transformation $\mathcal{U}_z$ diagonalizes $\mathcal{H}^{\mathrm{B}}$, we note that the latter can be written as

$$\mathcal{H}^{\mathrm{B}} = \sum_{p\in P_{\mathrm{B}}}(p^2 - \mu_0)a_{p,z}^* a_{p,z} + \frac{\varrho_0(\beta, N, L)}{2}\sum_{p\in P_{\mathrm{B}}}\hat{v}_N * \hat{f}_N(p)\left[2a_{p,z}^* a_{p,z} + a_{p,z}^* a_{-p,z}^* + a_{p,z}a_{-p,z}\right]. \tag{2.19}$$

Eq. (2.17) now follows from a standard computation that uses (2.14) and (2.19), see e.g. [11, Lemma 5.2]. □

Remark 2.2. It is worth noting that, although $\mathcal{H}^{\mathrm{B}}$ depends on $z \in \mathbb{C}$, the r.h.s. of (2.17) is independent of z. This is related to the fact that the z-dependence of $\mathcal{H}^{\mathrm{B}}$ is quite simple: all functions of the plane wave basis are multiplied by the same complex phase.

Next, we compute the 1-pdm and the pairing function of the state $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$.

Lemma 2.3. *The 1-pdm and the pairing function of the state $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$ with $G_{\mathrm{B}}(z)$ in (2.5) and G_{free} in (2.6) are for $p, q \in P_{\mathrm{B}} \cup P_{\mathrm{I}}$ given by*

$$\mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q^* a_p G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] = \delta_{p,q}\gamma(p) \quad \text{and} \quad \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_p a_q G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] = \delta_{p,-q}(z/|z|)^2\alpha(p), \tag{2.20}$$

respectively. Here

$$\begin{aligned}\gamma(p) &= \mathbb{1}(p \in P_{\mathrm{B}})\left((u_p^2 + v_p^2)\frac{1}{\exp(\beta\varepsilon(p)) - 1} + v_p^2\right) + \mathbb{1}(p \in P_{\mathrm{I}})\frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} \quad \text{and}\\ \alpha(p) &= \mathbb{1}(p \in P_{\mathrm{B}})u_p v_p\left(\frac{2}{\exp(\beta\varepsilon(p)) - 1} + 1\right)\end{aligned} \tag{2.21}$$

with $\varepsilon(p)$ in (2.18).

Proof. We start by noting that the special form of the 1-pdm and the pairing function in (2.20) follows immediately from the translation invariance of the state $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$. To compute $\gamma(p)$, we write

$$\mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q^* a_p G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] = \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[\mathcal{U}_z^* a_q^* a_p \mathcal{U}_z \mathcal{U}_z^* G_{\mathrm{B}}(z)\mathcal{U}_z \otimes G_{\mathrm{free}}]. \tag{2.22}$$

Using $a_p = (z/|z|)a_{p,z}$ and Lemma 2.1, we see that

$$\begin{aligned}\mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q^* a_p \mathcal{U}_z^* G_{\mathrm{B}}(z)\mathcal{U}_z] &= \delta_{p,q}\frac{1}{\exp(\beta\varepsilon(p) - 1},\\ \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q^* a_p^* \mathcal{U}_z^* G_{\mathrm{B}}(z)\mathcal{U}_z] &= 0 = \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q a_p \mathcal{U}_z^* G_{\mathrm{B}}(z)\mathcal{U}_z]\end{aligned} \tag{2.23}$$

holds for $p, q \in P_{\mathrm{B}}$. We also have

$$\begin{aligned}\mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q^* a_p G_{\mathrm{free}}] &= \delta_{p,q}\frac{1}{\exp(\beta(p^2 - \mu_0) - 1},\\ \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q^* a_p^* G_{\mathrm{free}}] &= 0 = \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}\otimes\mathscr{F}_{\mathrm{I}}}[a_q a_p G_{\mathrm{free}}],\end{aligned} \tag{2.24}$$

for $p, q \in P_{\mathrm{I}}$. Since $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$ is a quasi-free state we know that the expectations in (2.20) vanish if one momentum is in P_{B} and the other in P_{I}. When we use (2.14), $a_p = (z/|z|)a_{p,z}$, (2.23) and (2.24) on the r.h.s. of (2.22), we obtain the claimed formula for the 1-pdm. The formula for the pairing function follows from a similar computation. □

We highlight that the pairing function of $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$ depends on $z/|z|$, while the 1-pdm does not. We state now a result useful to estimate momentum sums. Its proof can be found in [25, Lemma 3.3].

Lemma 2.4. *Let $f : [0, \infty) \to \mathbb{R}$ be a nonnegative and monotone decreasing function and choose some $\kappa \geq 0$. Then*

$$\sum_{p \in \Lambda_+^*} f(|p|) \mathbb{1}(|p| \geq \kappa) \leq \left(\frac{L^3}{2\pi} \right) \int_{|p| \geq \left[\kappa - \sqrt{3}\frac{2\pi}{L}\right]_+} f(|p|) \left(1 + \frac{3\pi}{L|p|} + \frac{6\pi}{L^2 p^2} \right) \mathrm{d}p. \tag{2.25}$$

The next lemma provides us with bounds for the functions γ and α.

Lemma 2.5. *The functions γ and α in (2.20) satisfy the pointwise bounds*

$$\begin{aligned} \gamma(p) &\lesssim \mathbb{1}(p \in P_{\mathrm{L}} \backslash \{0\}) \frac{1}{\exp(\beta p^2) - 1} + \mathbb{1}(p \in P_{\mathrm{B}}) \frac{1}{L^4 p^4} \quad \textit{and} \\ |\alpha(q)| &\lesssim \mathbb{1}(p \in P_{\mathrm{B}}) \frac{1}{L^2 p^2} \left(1 + \frac{1}{\beta p^2} \right). \end{aligned} \tag{2.26}$$

Moreover, for $n \in \{0, 1\}$ we have

$$\begin{aligned} &\sum_{p \in \Lambda_+^*} |p|^1 \gamma(p) \lesssim L^3 \beta^{-(3+n)/2} + L^{-n} c_n(N) \quad \textit{with} \quad c_n(N) = \begin{cases} 1 & \textit{if } n = 0 \\ \ln(N) & \textit{if } n = 1 \end{cases} \quad \textit{as well as} \\ &\sum_{p \in \Lambda_+^*} |p|^n |\alpha(p)| \lesssim L^{-n+2} \beta^{-1} c_n(N) + L^{-n} N^{(n+1)\delta_{\mathrm{B}}}. \end{aligned} \tag{2.27}$$

Finally, the number of particles with momenta in P_{B} is bounded by

$$\sum_{p \in P_{\mathrm{B}}} \gamma(p) \lesssim 1 + \frac{L^2 N^{\delta_{\mathrm{B}}}}{\beta}. \tag{2.28}$$

Proof. We start by noting that

$$v_p^2 = \frac{1}{4} \left(\frac{p^2 - \mu_0}{p^2 - \mu_0 + 2\hat{v}_N * \hat{f}_N(p) \varrho_0} \right)^{1/2} + \frac{1}{4} \left(\frac{p^2 - \mu_0}{p^2 - \mu_0 + 2\hat{v}_N * \hat{f}_N(p) \varrho_0} \right)^{-1/2} - \frac{1}{2}. \tag{2.29}$$

As already remarked above, we can assume that $2\hat{v}_N * \hat{f}_N(p) \geq 0$ holds uniformly in $p \in P_{\mathrm{B}}$ (see (2.16)). In combination with the bound $0 \leq (1 + x)^{-1/2} + (1 + x)^{1/2} - 2 \leq x^2/4$ for $x \geq 0$ and $\mu_0 < 0$, this implies

$$v_p^2 \leq \frac{(\varrho_0 \hat{v}_N * \hat{f}_N(p))^2}{4p^4}. \tag{2.30}$$

Using $0 \leq f_N \leq 1$, we see that

$$|\hat{v}_N * \hat{f}_N(p)| \leq \int_\Lambda v_N(x) f_N(x) \, \mathrm{d}x \leq N^{-1} \int_\Lambda v(x) \, \mathrm{d}x, \tag{2.31}$$

and hence

$$v_p^2 \lesssim \frac{N_0^2}{N^2 L^4 p^4} \leq \frac{1}{L^4 p^4}. \tag{2.32}$$

The bounds for $\gamma(p)$ and $|\alpha(p)|$ now follow from (2.21), (2.32), $u_p^2 - v_p^2 = 1$ and $\varepsilon(p) \geq p^2 - \mu_0 \geq p^2$. The bounds in (2.27) and (2.28) are a direct consequence of the pointwise bounds for $\gamma(p)$ and $|\alpha(p)|$ and Lemma 2.4. $\square$

Properties of the state Γ_0

Recall definition (2.9) for $\widetilde{N}_0$, the expected number of particles in the condensate of our trial state Γ_0. We highlight that if we know $\widetilde{N}_0$ we can compute the chemical potential $\widetilde{\mu}$ in the definition of ζ, see the discussion below (2.7). In the following lemma, we prove a bound for $\widetilde{N}_0$ showing that it is close to N_0 in (1.12) in a suitable sense.

Lemma 2.6. *Assume that $\beta \gtrsim \beta_{\mathrm{c}}$. There exists a constant $c > 0$ such that $\widetilde{N}_0$ satisfies the bound*

$$|\widetilde{N}_0 - N_0| \lesssim \frac{N_0 L^2}{N\beta} + \frac{N_0^2}{N^2} + \exp(-cN^{2\delta_{\mathrm{L}}}). \tag{2.33}$$

Proof. The expected number of particles in the state Γ_0 equals N, that is,

$$N = \int_{\mathbb{C}} \mathrm{Tr}[\mathcal{N}\, |z\rangle\langle z| \otimes G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}]\zeta(z)\,\mathrm{d}z = \int_{\mathbb{C}} |z|^2 \zeta(z)\,\mathrm{d}z + \sum_{p\in\Lambda_+^*} \gamma(p), \tag{2.34}$$

where we used Lemma 2.3 to obtain the second identity. We apply Lemma 2.3 and the identity $u_p^2 - v_p^2 = 1$ to see that the part of the sum on the r.h.s. that runs over P_{B} can be written as

$$\sum_{p\in P_{\mathrm{B}}} \gamma(p) = \sum_{p\in P_{\mathrm{B}}} \frac{1}{\exp(\beta\varepsilon(p)) - 1} + 2\sum_{p\in P_{\mathrm{B}}} \frac{1}{\exp(\beta\varepsilon(p)) - 1} v_p^2 + \sum_{p\in P_{\mathrm{B}}} v_p^2 \tag{2.35}$$

with $\varepsilon(p)$ in (2.18) and v_p^2 in (2.29). We use $\varepsilon(p) \geq p^2$, $(\exp(x) - 1)^{-1} \leq 1/x$, and the bound for v_p^2 in (2.32) to see that the second term on the r.h.s. is bounded by

$$2\sum_{p\in P_{\mathrm{B}}} \frac{1}{\exp(\beta\varepsilon(p)) - 1} v_p^2 \lesssim \sum_{p\in\Lambda_+^*} \frac{1}{\beta p^2} \frac{N_0^2}{N^2 L^4 p^4} \lesssim \frac{N_0^2 L^2}{N^2 \beta}. \tag{2.36}$$

Moreover, for the third term

$$\sum_{p\in P_{\mathrm{B}}} v_p^2 \lesssim \frac{N_0^2}{N^2} \tag{2.37}$$

holds.

We also claim that

$$\left| \sum_{p\in P_{\mathrm{B}}} \left(\frac{1}{\exp(\beta\varepsilon(p)) - 1} - \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} \right) \right| \lesssim \frac{N_0 L^2}{N\beta}. \tag{2.38}$$

To see this, we write

$$\frac{1}{\exp(\beta\varepsilon(p)) - 1} = \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} - \int_0^1 \frac{\beta(p^2 - \mu_0)\left(\sqrt{1 + \frac{2\varrho_0 \hat{v}_N * f_N(p)}{p^2 - \mu_0}} - 1\right)}{4\sinh^2\left((t(p^2 - \mu_0) + (1 - t)\varepsilon(p))/2\right)}\,\mathrm{d}t. \tag{2.39}$$

Using $|\sqrt{1+x} - 1| \leq x/2$ for $x \geq 0$ and (2.31), we check that

$$\left| \sqrt{1 + \frac{2\varrho_0 \hat{v}_N * f_N(p)}{p^2 - \mu_0}} - 1 \right| \leq \frac{\varrho_0 \hat{v}_N * f_N(p)}{p^2 - \mu_0} \leq \frac{2\varrho_0 \|v\|_1}{N(p^2 - \mu_0)} \lesssim \frac{N_0}{NL^2(p^2 - \mu_0)}. \tag{2.40}$$

In combination, (2.39), (2.40), $\varepsilon(p) \geq p^2 - \mu_0$ and $\mu_0 < 0$ imply

$$\left| \sum_{p \in P_{\mathrm{B}}} \left(\frac{1}{\exp(\beta\varepsilon(p)) - 1} - \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} \right) \right| \lesssim \frac{N_0 \beta}{N L^2} \sum_{p \in P_{\mathrm{B}}} \frac{1}{\sinh^2(\beta(p^2 - \mu_0)/2)} \leq \frac{N_0}{N \beta L^2} \sum_{p \in \Lambda_+^*} \frac{1}{p^4}, \tag{2.41}$$

which proves (2.38).

When we put (2.34)–(2.37) and (2.38) together and use (2.21), we find

$$N = \widetilde{N}_0 + \sum_{p \in P_{\mathrm{L}} \backslash \{0\}} \frac{1}{\exp(\beta(p^2 - \mu_0))} + O\left(\frac{N_0 L^2}{N \beta} \right) \tag{2.42}$$

with $\widetilde{N}_0$ in (2.9). The second term on the r.h.s. can be written as

$$\sum_{p \in P_{\mathrm{L}} \backslash \{0\}} \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} = \sum_{p \in \Lambda_+^*} \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} - \sum_{p \in P_{\mathrm{L}}^{\mathrm{c}}} \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1}, \tag{2.43}$$

where $P_{\mathrm{L}}^{\mathrm{c}}$ denotes the complement of the set P_{L}. The first term on the r.h.s. equals $N - N_0$ with N_0 in (1.12) and the second term satisfies the bound

$$\sum_{p \in P_{\mathrm{L}}^{\mathrm{c}}} \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} \leq \left(\frac{1}{\exp\left(\beta N^{2/3 + 2\delta_{\mathrm{L}}}\right) - 1} \right)^{1/2} \sum_{p \in \Lambda_+^*} \left(\frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} \right)^{1/2} \lesssim \exp(-c N^{2\delta_{\mathrm{L}}}) N \tag{2.44}$$

for some $c > 0$. To obtain (2.44), we used $\beta \gtrsim \beta_{\mathrm{c}}$ and the definition of P_{L} in (2.1). When we put (2.42)–(2.44) together, and use the assumption $\delta_{\mathrm{L}} > 0$, we obtain a proof of (2.33). □

For the computation of the energy of Γ_0 we need to know its 2-particle density matrix (2-pdm), which is stated in the next lemma.

Lemma 2.7. *The 2-pdm of the state Γ_0 in (2.7) reads*

$$\begin{aligned} \mathrm{Tr}_{\mathscr{F}} \left[a_{u_1}^* a_{v_1}^* a_{u_2} a_{v_2} \Gamma_0 \right] = {} & \delta_{u_1,0} \delta_{v_1,0} \delta_{u_2,0} \delta_{v_2,0} \int_{\mathbb{C}} |z|^4 \zeta(z) \, \mathrm{d}z \\ & + \widetilde{N}_0 \left[\gamma(v_1) \delta_{v_1,v_2} \delta_{u_1,0} \delta_{u_2,0} + \gamma(u_1) \delta_{u_1,u_2} \delta_{v_1,0} \delta_{v_2,0} + \gamma(u_1) \delta_{u_1,v_2} \delta_{v_1,0} \delta_{u_2,0} + \gamma(v_1) \delta_{v_1,u_2} \delta_{u_1,0} \delta_{v_2,0} \right] \\ & + \widetilde{N}_0 \left[\alpha(u_2) \delta_{u_2,-v_2} \delta_{u_1,0} \delta_{v_1,0} + \overline{\alpha(u_1)} \delta_{u_1,-v_1} \delta_{u_2,0} \delta_{v_2,0} \right] \\ & + \gamma(u_1) \gamma(v_1) \delta_{u_1,u_2} \delta_{v_1,v_2} + \gamma(u_1) \gamma(v_1) \delta_{u_1,v_2} \delta_{v_1,u_2} + \overline{\alpha(u_1)} \alpha(u_2) \delta_{u_1,-v_1} \delta_{u_2,-v_2} \end{aligned} \tag{2.45}$$

with $\widetilde{N}_0$ in (2.9) and γ, α in (2.21).

Proof. We denote by $\mathcal{W}_z = \exp(z a_0^* - \bar{z} a_0)$ the Weyl transformation that implements the condensate. Using $\mathcal{W}_z^* a_0 \mathcal{W}_z = a_0 + z$, we find

$$\mathrm{Tr}_{\mathscr{F}} [a_{u_1}^* a_{v_1}^* a_{u_2} a_{v_2} \Gamma_0] = \int_{\mathbb{C}} \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [A_{u_1,v_1,u_2,v_2} G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] \zeta(z) \, \mathrm{d}z \tag{2.46}$$

with the operator

$$\begin{aligned} A_{u_1,v_1,u_2,v_2} = {} & |z|^4 \delta_{u_1,0} \delta_{v_1,0} \delta_{u_2,0} \delta_{v_2,0} \\ & + |z|^2 \Big(a_{v_1}^* a_{v_2} \delta_{u_1,0} \delta_{u_2,0} + a_{u_1}^* a_{u_2} \delta_{v_1,0} \delta_{v_2,0} + a_{u_1}^* a_{v_2} \delta_{v_1,0} \delta_{u_2,0} + a_{v_1}^* a_{u_2} \delta_{u_1,0} \delta_{v_2,0} \Big) \\ & + \bar{z}^2 a_{u_2} a_{v_2} \delta_{u_1,0} \delta_{v_1,0} + z^2 a_{u_1}^* a_{v_1}^* \delta_{u_2,0} \delta_{v_2,0} + a_{u_1}^* a_{v_1}^* a_{u_2} a_{v_2}. \end{aligned} \tag{2.47}$$

An application of Lemma 2.3 allows us to compute the terms proportional to $|z|^2$, z^2 and $\overline{z}^2$. It remains to compute the expectation of the last term in (2.47). Since $G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}$ is a quasi-free state we can apply the Wick theorem and find

$$\begin{aligned} \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] = {} & \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{u_1} a_{u_2} G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{v_1} a_{v_2} G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] \\ & + \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{u_1} a_{v_2} G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{v_1} a_{u_2} G_{\mathrm{B}}(z) \otimes G_{\mathrm{free}}] \\ & + \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}}} [a^*_{u_1} a^*_{v_1} G_{\mathrm{B}}(z)] \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}}} [a_{u_2} a_{v_2} G_{\mathrm{B}}(z)]. \end{aligned} \tag{2.48}$$

The claimed identity in (2.45) follows when we apply Lemma 2.3 to compute the expectations in (2.48). □

Our last preparatory lemma contains bounds for the 2, 3 and 4-pdms of Γ_0.

Lemma 2.8. *The state Γ_0 in (2.7) satisfies*

$$\begin{aligned} \sum_{\substack{u_1, v_1 \in P_{\mathrm{L}} \\ u_2, v_2 \in P_{\mathrm{L}}}} \left| \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{u_1} a^*_{v_1} a_{u_2} a_{v_2} \Gamma_0] \right| &\lesssim N^2, \\ \sum_{\substack{u_1, u_2, u_3 \in P_{\mathrm{L}} \\ v_1, v_2, v_3 \in P_{\mathrm{L}}}} \left| \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{v_1} a^*_{v_2} a^*_{v_3} a_{u_1} a_{u_2} a_{u_3} \Gamma_0] \right| &\lesssim N^3, \quad \textit{and} \\ \sum_{\substack{u_1, u_2, u_3, u_4 \in P_{\mathrm{L}} \\ v_1, v_2, v_3, v_4 \in P_{\mathrm{L}}}} \left| \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}} \otimes \mathscr{F}_{\mathrm{I}}} [a^*_{v_1} a^*_{v_2} a^*_{v_3} a^*_{v_4} a_{u_1} a_{u_2} a_{u_3} a_{u_4} \Gamma_0] \right| &\lesssim N^4. \end{aligned} \tag{2.49}$$

Proof. The first bound is a direct consequence of Lemma 2.5 and Lemma 2.7. To prove the second and the third bound we first need to compute the 3-pdm and the 4-pdm of Γ_0 as in the proof of Lemma 2.7. Afterwards, applications of Lemma 2.5 and Lemma C.3 prove the claim. Carrying out these steps is straightforward but a little lengthy. We therefore leave the details to the reader. □

3. Bound for the energy

We compute now the expectation of the Hamiltonian $\mathcal{H}_N$, defined in (1.5) and (1.3), on our trial state. The main result of this section is Proposition 3.1 below. This, together with Proposition 4.1 for the entropy contribution (in Section 4) will be the main ingredient to prove Theorem 1.1.

Proposition 3.1. *Assume that $v : [0, \infty) \to [0, \infty]$ is nonnegative, compactly supported, and satisfies $v(|\cdot|) \in L^3(\Lambda, \mathrm{d}x)$. Let Γ be defined in (2.13) and $\beta = \kappa \beta_{\mathrm{c}}$, with $\kappa \in (0, \infty)$. Then we have*

$$\operatorname{Tr}[\mathcal{H}_N \Gamma] - E_{\mathcal{H}_N} \lesssim L^{-2} \mathcal{E}_{\mathcal{H}_N} \tag{3.1}$$

where

$$\begin{aligned} E_{\mathcal{H}_N} = {} & \operatorname{Tr}_{\mathscr{F}_{\mathrm{I}}} \Big[\Big(\sum_{p \in P_{\mathrm{I}}} p^2 a^*_p a_p \Big) G_{\mathrm{free}} \Big] \\ & + \operatorname{Tr}_{\mathscr{F}_{\mathrm{B}}} \Big[\sum_{p \in P_{\mathrm{B}}} \Big(p^2 a^*_p a_p + \frac{N_0(\beta, N, L)}{2|\Lambda|} (\hat{v}_N * \hat{f}_N)(p) \big(2\, a^*_p a_p + (z^2/|z|^2) a^*_p a^*_{-p} + (\overline{z}^2/|z|^2) a_p a_{-p} \big) \Big) G_{\mathrm{B}}(z) \Big] \\ & + \frac{4\pi \mathfrak{a}}{N|\Lambda|} \Big[\int_{\mathbb{C}} |z|^4 \zeta(z) \, \mathrm{d}z + 2\widetilde{N}_0 \sum_{u \in P_{\mathrm{L}} \setminus \{0\}} \gamma(u) + 2\widetilde{N}_0 \sum_{q \in P_{\mathrm{I}}} \gamma(q) + 2 \sum_{u, v \in P_{\mathrm{L}} \setminus \{0\}} \gamma(v) \gamma(u) \Big] \end{aligned} \tag{3.2}$$

and

$$\mathcal{E}_{\mathcal{H}_N} = N^{1-\delta_{\mathrm{H}}} + N^{\delta_{\mathrm{H}} + 2\delta_{\mathrm{B}}} + N^{-1/3 + \delta_{\mathrm{H}} + 2\delta_L} + N^{1/3 + \delta_{\mathrm{B}}}. \tag{3.3}$$

The parameter $\widetilde{N}_0$ has been introduced in (2.9), while $N_0(\beta, N, L)$ has been defined in (1.12).

Remark 3.2. The z-dependence of the Bogoliubov Hamiltonian and of $G_{\mathrm{B}}(z)$ in the second line of (3.2) cancel out exactly. This explains why this term is not integrated over z.

To prove Proposition 3.1, we split the Hamiltonian in two contributions: we define

$$\mathcal{K} = \sum_{p\in\Lambda_+^*} p^2 a_p^* a_p \qquad \text{and} \qquad \mathcal{V}_N = \frac{1}{2|\Lambda|} \sum_{p,u,v\in\Lambda^*} \hat{v}_N(p)\, a_{u+p}^* a_{v-p}^* a_u a_v \tag{3.4}$$

so that $\mathcal{H}_N = \mathcal{K} + \mathcal{V}_N$. We have therefore

$$\mathrm{Tr}\,[\mathcal{H}_N\Gamma] = \sum_\alpha \lambda_\alpha \frac{\langle (1+B)\psi_\alpha, (\mathcal{K}+\mathcal{V}_N)(1+B)\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle} =: \mathcal{G}_{\mathcal{K}} + \mathcal{G}_{\mathcal{V}}. \tag{3.5}$$

We will prove Proposition 3.1 in Section 3.3, using the results of Lemma 3.3 below for the analysis of $\mathcal{G}_{\mathcal{V}}$ and Lemma 3.4 for the analysis of $\mathcal{G}_{\mathcal{K}}$.

3.1. Analysis of $\mathcal{G}_{\mathcal{V}}$

In this section we prove an upper bound for $\mathcal{G}_{\mathcal{V}}$, as stated in the following lemma.

Lemma 3.3. *Under the assumptions of Proposition 3.1, we have*

$$\mathcal{G}_V - E_{\mathcal{V}_N} \lesssim L^{-2}(N^{1-\delta_{\mathrm{H}}} + N^{1/3} + N^{\delta_{\mathrm{H}}}), \tag{3.6}$$

where

$$\begin{aligned} E_{\mathcal{V}_N} =& \frac{4\pi\mathfrak{a}}{N|\Lambda|}\int_{\mathbb{C}} |z|^4 \zeta(z)\,\mathrm{d}z + \frac{8\pi\mathfrak{a}\widetilde{N}_0}{N|\Lambda|}\sum_{u\in P_{\mathrm{L}}\setminus\{0\}} \gamma(u) \\ &+ \frac{\widetilde{N}_0}{2|\Lambda|^2}\sum_{p,q\in\Lambda^*} \hat{v}_N(p-q)\hat{f}_N(p)\Big[2\gamma(q) + \alpha(q) + \overline{\alpha(q)}\Big] + \frac{8\pi\mathfrak{a}}{N|\Lambda|}\sum_{u,v\in P_{\mathrm{L}}\setminus\{0\}} \gamma(v)\gamma(u) \\ &+ \frac{1}{2|\Lambda|^2}\sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2,v_2\in P_{\mathrm{L}}}} \eta_{p_1}\Big[\hat{v}_N(p_1+u_1-u_2) + \frac{1}{|\Lambda|}\sum_{p_2\in P_{\mathrm{H}}} \hat{v}_N(p_1+p_2+u_1-u_2)\eta_{p_2}\Big]\mathrm{Tr}[a_{v_1}^* a_{u_1}^* a_{v_2} a_{u_2}\Gamma_0]. \end{aligned} \tag{3.7}$$

The functions $\gamma(p)$ and $\alpha(p)$ are defined in (2.21).

Proof. Recall definition (2.12) for B. Acting on ψ_α (i.e., the eigenfunctions of Γ_0, defined in (2.7)) with annihilation operators of momenta in P_{H} gives zero. Therefore $\langle\psi_\alpha, B\,\psi_\alpha\rangle = \langle\psi_\alpha, B^*\,\psi_\alpha\rangle = 0$, and we can estimate the denominator in (3.8) as $\|(1+B)\psi_\alpha\|^2 = \langle\psi_\alpha,(1+B^*B)\,\psi_\alpha\rangle \geq 1$ so to have the upper bound

$$\mathcal{G}_V \leq \sum_\alpha \lambda_\alpha\,\langle\psi_\alpha, \mathcal{V}_N(1+B)\psi_\alpha\rangle + \sum_\alpha \lambda_\alpha\,\langle\psi_\alpha, B^*\mathcal{V}_N(1+B)\psi_\alpha\rangle =: \mathcal{G}_V^{(1)} + \mathcal{G}_V^{(2)}. \tag{3.8}$$

With definitions (3.4) for $\mathcal{V}_N$ and (2.12) for B we write

$$\begin{aligned} \mathcal{G}_V^{(1)} &= \mathrm{Tr}[\mathcal{V}_N(1+B)\Gamma_0] = \frac{1}{2|\Lambda|}\sum_{p_1,u_1,v_1\in\Lambda^*} \hat{v}_N(p_1)\ \mathrm{Tr}[a_{u_1+p_1}^* a_{v_1-p_1}^* a_{u_1} a_{v_1}\Gamma_0] \\ &\quad + \frac{1}{4|\Lambda|^2}\sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in P_{\mathrm{H}},\,u_2,v_2\in P_{\mathrm{L}}}} \hat{v}_N(p_1)\eta_{p_2}\ \mathrm{Tr}[a_{u_1+p_1}^* a_{v_1-p_1}^* a_{u_1} a_{v_1} a_{u_2+p_2}^* a_{v_2-p_2}^* a_{u_2} a_{v_2}\Gamma_0] \\ &=: \mathcal{G}_V^{(1,1)} + \mathcal{G}_V^{(1,2)}. \end{aligned} \tag{3.9}$$

Using the commutation relations (2.3), we bring the monomial $a_{u_1}a_{v_1}a^*_{u_2+p_2}a^*_{v_2-p_2}$ in $\mathcal{G}_V^{(1,2)}$ to normal order. When we exploit again that acting on Γ_0 with annihilation operators of momenta in $P_{\rm H}$ gives zero, we remain with

$$\mathcal{G}_V^{(1,2)} = \frac{1}{2|\Lambda|^2} \sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in P_{\rm H},\, u_2,v_2\in P_{\rm L}}} \hat{v}_N(p_1)\eta_{p_2}\ \mathrm{Tr}[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_2}a_{v_2}\Gamma_0]\delta_{v_1,v_2-p_2}\delta_{u_1,u_2+p_2}, \tag{3.10}$$

where in addition we used the symmetry under exchange of u_1 with v_1 and p_1 with $-p_1$. We add and subtract the contributions where $p_2 \in P_{\rm H}^{\rm c} = \{p \in \Lambda^* \mid |p| < N^{1-\delta_{\rm H}}/L\}$; using the definition of η_p in (2.11) we find

$$\begin{aligned}
\mathcal{G}_V^{(1,2)} = &-\frac{1}{2|\Lambda|} \sum_{p_1,u_1,v_1\in\Lambda^*} \hat{v}_N(p_1)\ \mathrm{Tr}[a^*_{u_1+p_1}a^*_{v_1-p_1}a_{u_1}a_{v_1}\Gamma_0] \\
&+ \frac{1}{2|\Lambda|^2} \sum_{\substack{p_1\in\Lambda^*\\ p_2\in\Lambda^*,\, u_2,v_2\in P_{\rm L}}} \hat{v}_N(p_1)\hat{f}_N(p_2)\ \mathrm{Tr}[a^*_{u_2+p_2+p_1}a^*_{v_2-p_2-p_1}a_{u_2}a_{v_2}\Gamma_0] \\
&+ \frac{1}{2|\Lambda|^2} \sum_{\substack{p_1,u_1,v_1\in\Lambda^*\\ p_2\in P_{\rm H}^{\rm c},\, u_2,v_2\in P_{\rm L}}} \hat{v}_N(p_1)\eta_{p_2}\ \mathrm{Tr}[a^*_{u_2+p_2+p_1}a^*_{v_2-p_2-p_1}a_{u_2}a_{v_2}\Gamma_0]
\end{aligned} \tag{3.11}$$

The first contribution in (3.11) cancels with the first contribution in (3.9). In the following, we denote the second and the third term on the r.h.s. of (3.11) by $\tilde{\mathcal{G}}_V$ and $\mathcal{E}_V^{(1)}$, respectively.

Using Lemma 2.8 to estimate the trace, equation (A.9) to estimate the sum of η_{p_2} over p_2 and the bound $|\hat{v}_N(p_1)| \leq \int v_N(x)\,\mathrm{d}x \lesssim LN^{-1}$, we see that

$$|\mathcal{E}_V^{(1)}| \leq \frac{1}{2|\Lambda|^2}\Big[\sup_{p_1\in\Lambda^*} |\hat{v}_N(p_1)|\Big] \sum_{p_2\in P_{\rm H}^{\rm c}} |\eta_{p_2}| \sum_{p_1\in\Lambda^*,u_2,v_2\in P_{\rm L}} \big|\mathrm{Tr}[a^*_{u_2+p_2+p_1}a^*_{v_2-p_2-p_1}a_{u_2}a_{v_2}\Gamma_0]\big| \lesssim L^{-2}N^{1-\delta_{\rm H}}. \tag{3.12}$$

We consider now $\tilde{\mathcal{G}}_V$; we compute the trace using Lemma 2.7 and obtain

$$\begin{aligned}
\tilde{\mathcal{G}}_V = \frac{1}{2|\Lambda|^2} \sum_{p_1,p_2\in\Lambda^*} \hat{v}_N(p_1)\hat{f}_N(p_2)\Big[&\delta_{p_1+p_2,0}\int_{\mathbb{C}} |z|^4\,\zeta(z)\,\mathrm{d}z + 2\widetilde{N}_0\delta_{p_1+p_2,0}\sum_{u\in P_{\rm L}\setminus\{0\}}\gamma(u) + 2\widetilde{N}_0\gamma(p_1+p_2) \\
&+ \widetilde{N}_0\alpha(p_1+p_2) + \widetilde{N}_0\overline{\alpha(p_1+p_2)} + \sum_{u\in P_{\rm B}\setminus\{0\}} \overline{\alpha(u+p_2+p_1)}\alpha(u) \\
&+ \delta_{p_1+p_2,0}\sum_{u,v\in P_{\rm L}\setminus\{0\}}\gamma(v)\gamma(u) + \sum_{u\in P_{\rm L}\setminus\{0\}}\gamma(u+p_2+p_1)\gamma(u)\Big] =: \sum_{j=1}^{8}\tilde{\mathcal{G}}_{V,j}.
\end{aligned} \tag{3.13}$$

Using (A.3) we see that

$$\sum_{p\in\Lambda^*} \hat{v}_N(p)\hat{f}_N(p) = \frac{|\Lambda|}{N}\int v(x)f(x)\,\mathrm{d}x = \frac{|\Lambda|}{N}\,(8\pi\mathfrak{a} + CL/N)\,, \tag{3.14}$$

and therefore the first contribution in (3.13) satisfies

$$\tilde{\mathcal{G}}_{V,1} = \frac{1}{2|\Lambda|^2}\sum_{p\in\Lambda^*}\hat{v}_N(p)\hat{f}_N(p)\int_{\mathbb{C}}|z|^4\zeta(z)\,\mathrm{d}z \leq \frac{4\pi\mathfrak{a}}{N|\Lambda|}\int_{\mathbb{C}}|z|^4\zeta(z)\,\mathrm{d}z + CL^{-2}. \tag{3.15}$$

To obtain a bound for the integral over $|z|^4$ we applied Lemma C.3.

We consider now $\tilde{\mathcal{G}}_{V,2}$. From $\sum_{u\in\Lambda_+^*}\gamma(u)\le N$ and (3.14) we know that

$$\tilde{\mathcal{G}}_{V,2}=\frac{\widetilde{N}_0}{|\Lambda|^2}\sum_{p\in\Lambda^*}\hat{v}_N(p)\hat{f}_N(p)\sum_{u\in P_{\rm L}\setminus\{0\}}\gamma(u)\le\frac{8\pi\mathfrak{a}\widetilde{N}_0}{N|\Lambda|}\sum_{u\in P_{\rm L}\setminus\{0\}}\gamma(u)+CL^{-2}\tag{3.16}$$

holds. The sum of $\tilde{\mathcal{G}}_{V,3},\tilde{\mathcal{G}}_{V,4}$ and $\tilde{\mathcal{G}}_{V,5}$ is left untouched, i.e.,

$$\tilde{\mathcal{G}}_{V,3}+\tilde{\mathcal{G}}_{V,4}+\tilde{\mathcal{G}}_{V,5}=\frac{\widetilde{N}_0}{2|\Lambda|^2}\sum_{p,q\in\Lambda^*}\hat{v}_N(p-q)\hat{f}_N(p)\big[2\gamma(q)+\alpha(q)+\overline{\alpha(q)}\big].\tag{3.17}$$

Next, we consider $\tilde{\mathcal{G}}_{V,6}$; from (A.3) it follows that

$$\sup_{p\in\Lambda^*}\Big|\sum_{q\in\Lambda^*}\hat{v}_N(q)\hat{f}_N(p-q)\Big|\le\frac{|\Lambda|}{N}\Big(8\pi\mathfrak{a}+\frac{CL}{N}\Big);\tag{3.18}$$

using in addition (2.27) and $\delta_{\rm B}<1/3$ we see that

$$|\tilde{\mathcal{G}}_{V,6}|=\frac{1}{2|\Lambda|^2}\Big|\sum_{p,q\in\Lambda^*}\hat{v}_N(q)\hat{f}_N(p-q)\sum_{u\in P_{\rm B}\setminus\{0\}}\bar{\alpha}(u+p)\alpha(u)\Big|\le CL^{-2}N^{1/3}.\tag{3.19}$$

Using (3.14) and (3.18) we see that the last two terms in (3.13) are equal at leading order:

$$\begin{aligned}\tilde{\mathcal{G}}_{V,7}+\tilde{\mathcal{G}}_{V,8}&=\frac{1}{2|\Lambda|^2}\sum_{p\in\Lambda^*}\hat{v}_N(p)\hat{f}_N(p)\sum_{u,v\in P_{\rm L}\setminus\{0\}}\gamma(v)\gamma(u)+\frac{1}{2|\Lambda|^2}\sum_{p,q\in\Lambda^*}\hat{v}_N(q)\hat{f}_N(p-q)\sum_{u\in P_{\rm L}\setminus\{0\}}\gamma(u+p)\gamma(u)\\&\le\frac{8\pi\mathfrak{a}}{N|\Lambda|}\sum_{u,v\in P_{\rm L}\setminus\{0\}}\gamma(v)\gamma(u)+CL^{-2}.\end{aligned}\tag{3.20}$$

It remains to consider $\mathcal{G}_V^{(2)}$ in (3.8).

To that end, we write

$$\mathcal{G}_V^{(2)}=\operatorname{Tr}[B^*\mathcal{V}_N(1+B)\Gamma_0]=\operatorname{Tr}[B^*\mathcal{V}_N\Gamma_0]+\operatorname{Tr}[B^*\mathcal{V}_NB\Gamma_0]=:\mathcal{G}_V^{(2,1)}+\mathcal{G}_V^{(2,2)}.\tag{3.21}$$

We have

$$B^*\mathcal{V}_N=\frac{1}{4|\Lambda|^2}\sum_{\substack{p_1\in P_{\rm H}\\u_1,v_1\in P_L}}\eta_{p_1}\sum_{p_2,u_2,v_2\in\Lambda^*}\hat{v}_N(p_2)\,a^*_{v_1}a^*_{u_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{v_2}a_{u_2};\tag{3.22}$$

commuting $a_{u_1+p_1}a_{v_1-p_1}$ to the right and observing that only the contributions with $v_2,u_2\in P_{\rm L}$ give a non zero contribution, we arrive at

$$\begin{aligned}\mathcal{G}_V^{(2,1)}&=\frac{1}{2|\Lambda|^2}\sum_{\substack{p_1\in P_{\rm H}\\u_1,v_1\in P_{\rm L}}}\eta_{p_1}\sum_{\substack{p_2\in\Lambda^*\\u_2,v_2\in P_{\rm L}}}\hat{v}_N(p_2)\,\operatorname{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0]\delta_{u_2+p_2,u_1+p_1}\delta_{v_2-p_2,v_1-p_1}\\&=\frac{1}{2|\Lambda|^2}\sum_{\substack{p_1\in P_{\rm H}\\u_1,v_1,u_2,v_2\in P_{\rm L}}}\eta_{p_1}\hat{v}_N(p_1+u_1-u_2)\,\operatorname{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0]\delta_{v_2,u_1+v_1-u_2}.\end{aligned}\tag{3.23}$$

This term contributes to (3.7). Note that $\delta_{v_2,u_1+v_1-u_2}$ can be dropped here because Γ_0 is translation invariant.

To compute $\mathcal{G}_V^{(2,2)}$ we need to study

$$B^*\mathcal{V}_NB=\frac{1}{8|\Lambda|^3}\sum_{\substack{p_1,p_3\in P_{\rm H}\\u_1,v_1,u_3,v_3\in P_L\\p_2,u_2,v_2,\in\Lambda^*}}\eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,a^*_{v_1}a^*_{u_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{v_2}a_{u_2}a^*_{u_3+p_3}a^*_{v_3-p_3}a_{v_3}a_{u_3}.\tag{3.24}$$

We bring the monomial $a_{v_2}a_{u_2}a^*_{u_3+p_3}a^*_{v_3-p_3}$ to normal order; the symmetries under exchange of u_2 with v_2, of u_3 with v_3 and $\eta_{-p_2} = \eta_{p_2}$ allow to organize the result of the commutation in the following three contributions:

$$\mathcal{G}_V^{(2,2)} = \mathrm{J}_1 + \mathrm{J}_2 + \mathrm{J}_3 \tag{3.25}$$

with

$$\begin{aligned}
\mathrm{J}_1 &:= \frac{1}{8|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_\mathrm{H}\\ u_1,v_1,u_3,v_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a^*_{u_3+p_3}a^*_{v_3-p_3}a_{v_2}a_{u_2}a_{v_3}a_{u_3}\Gamma_0],\\
\mathrm{J}_2 &:= \frac{1}{2|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_\mathrm{H}\\ u_1,v_1,u_3,v_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a^*_{u_3+p_3}a_{u_2}a_{v_3}a_{u_3}\Gamma_0]\delta_{v_2,v_3-p_3},\\
\mathrm{J}_3 &:= \frac{1}{4|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_\mathrm{H}\\ u_1,v_1,u_3,v_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{v_3}a_{u_3}\Gamma_0]\delta_{u_2,v_3-p_3}\delta_{v_2,u_3+p_3}.
\end{aligned} \tag{3.26}$$

In J_1 we bring the monomial $a_{u_1+p_1}a_{v_1-p_1}a^*_{u_3+p_3}a^*_{v_3-p_3}$ to normal order; using that we obtain zero when we act with annihilations operators of momenta in P_H on Γ_0 and exploiting the symmetry under exchange of v_1 and u_1 we obtain

$$\mathrm{J}_1 = \frac{1}{4|\Lambda|^3} \sum_{\substack{p_1\in P_\mathrm{H}\\ u_1,v_1,u_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_1+u_1-u_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{v_2}a_{u_2}a_{v_1+u_1-u_3}a_{u_3}\Gamma_0]. \tag{3.27}$$

When we apply Lemma 2.8 and the Cauchy-Schwarz inequality, and use the bound in (A.8) as well as $|\hat{v}_N(p)| \lesssim LN^{-1}$, we see that

$$|\mathrm{J}_1| \lesssim \frac{L}{N|\Lambda|^3} \sum_{\substack{u_1,v_1,u_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \left|\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{v_2}a_{u_2}a_{v_1+u_1-u_3}a_{u_3}\Gamma_0]\right| \sum_{p_1\in P_\mathrm{H}} |\eta_{p_1}\eta_{p_1+u_1-u_3}| \lesssim L^{-2}N^{\delta_\mathrm{H}} \tag{3.28}$$

holds.

In J_2 we bring the monomial $a_{u_1+p_1}a_{v_1-p_1}a^*_{u_3+p_3}$ to normal order (so we obtain zero when $a^*_{u_3+p_3}$ acts on Γ_0, since $u_3+p_3\in P_\mathrm{H}$) and find

$$\mathrm{J}_2 = \frac{1}{|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_\mathrm{H}\\ u_1,v_1,u_3,v_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{u_2}a_{v_3}a_{u_3}\Gamma_0]\delta_{v_2,v_3-p_3}\delta_{u_1+p_1,u_3+p_3} \tag{3.29}$$

Now we normal order $a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}$ (with the aim of commuting $a_{v_1-p_1}$ to the right, since $v_1-p_1\in P_\mathrm{H}$) obtaining

$$\begin{aligned}
\mathrm{J}_2 &= \frac{2}{|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_\mathrm{H}\\ u_1,v_1,u_3,v_3\in P_\mathrm{L}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a^*_{u_2+p_2}a_{u_2}a_{v_3}a_{u_3}\Gamma_0]\delta_{v_2,v_3-p_3}\delta_{u_1+p_1,u_3+p_3}\delta_{v_1-p_1,v_2-p_2}\\
&= \frac{2}{|\Lambda|^3} \sum_{\substack{p_1\in P_\mathrm{H}\\ u_1,v_1,u_3,v_3,u_2\in P_\mathrm{L}}} \eta_{p_1}\hat{v}_N(v_3+u_3-v_1-u_1)\eta_{p_1+u_1-u_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a^*_{u_2-v_1+v_3-u_1+u_3}a_{u_2}a_{v_3}a_{u_3}\Gamma_0].
\end{aligned} \tag{3.30}$$

Again we exploited that v_1 can be exchanged with u_1 and v_2 with u_2. Using Lemma 2.8, (A.8) and $|\hat{v}_N(p)| \lesssim LN^{-1}$, we obtain the bound

$$|\mathrm{J}_2| \lesssim L^{-2}N^{-1+\delta_{\mathrm{H}}}. \tag{3.31}$$

Normal ordering of $a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}$ and analogous considerations as above lead to

$$\begin{aligned}
\mathrm{J}_3 &= \frac{1}{2|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_{\mathrm{H}}\\ u_1,v_1,u_3,v_3\in P_{\mathrm{L}}\\ p_2,u_2,v_2,\in\Lambda^*}} \eta_{p_1}\hat{v}_N(p_2)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_3}a_{u_3}\Gamma_0]\delta_{u_2,v_3-p_3}\delta_{v_2,u_3+p_3}\delta_{v_1-p_1,v_2-p_2}\delta_{u_2+p_2,u_1+p_1}\\
&= \frac{1}{2|\Lambda|^3} \sum_{\substack{p_1,p_3\in P_{\mathrm{H}}\\ u_1,v_1,v_3,u_3\in P_{\mathrm{L}}}} \eta_{p_1}\hat{v}_N(p_1+p_3+u_3-v_1)\eta_{p_3}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_3}a_{u_3}\Gamma_0].
\end{aligned} \tag{3.32}$$

We combine J_3 with $\mathcal{G}_V^{(2,1)}$ in (3.23) and obtain

$$\begin{aligned}
\mathcal{G}_V^{(2,1)}+\mathrm{J}_3 &= \frac{1}{2|\Lambda|^2} \sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,v_2,u_2\in P_{\mathrm{L}}}} \eta_{p_1}\hat{v}_N(p_1+u_1-u_2)\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0]\\
&\quad+\frac{1}{2|\Lambda|^3} \sum_{\substack{p_1,p_2\in P_{\mathrm{H}}\\ u_1,v_1,v_2,u_2\in P_{\mathrm{L}}}} \eta_{p_1}\hat{v}_N(p_1+p_2+u_2-v_1)\eta_{p_2}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0]\\
&=\frac{1}{2|\Lambda|^2} \sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2,v_2\in P_{\mathrm{L}}}} \eta_{p_1}\Big[\hat{v}_N(p_1+u_1-u_2)+\frac{1}{|\Lambda|}\sum_{p_2\in P_{\mathrm{H}}}\hat{v}_N(p_1+p_2+u_1-u_2)\eta_{p_2}\Big]\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0].
\end{aligned} \tag{3.33}$$

In the last line we used the symmetry under exchange of v_1 with u_1. Collecting the results of (3.8), (3.15), (3.16), (3.17), (3.20), (3.21), (3.25), (3.33) and the bounds on the error terms in (3.12), (3.19), (3.28), (3.31) we obtain (3.6). □

3.2. Analysis of $\mathcal{G}_{\mathcal{K}}$

We recall from definitions of $\mathcal{K}$ in (3.4) and $\mathcal{G}_{\mathcal{K}}$ in (3.5). In this section we prove an upper bound for $\mathcal{G}_{\mathcal{K}}$, as stated in the following lemma.

Lemma 3.4. *Under the assumptions of Proposition 3.1 we have*

$$\mathcal{G}_{\mathcal{K}} - E_{\mathcal{K}} \lesssim L^{-2}(N^{\delta_{\mathrm{H}}+2\delta_{\mathrm{B}}} + N^{-1/3+\delta_{\mathrm{H}}+2\delta_L} + N^{1/3}\ln(N)) \tag{3.34}$$

with

$$E_{\mathcal{K}} = \sum_{p\in P_{\mathrm{L}}} p^2\gamma(p) + \frac{1}{|\Lambda|^2}\sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2,v_2\in P_{\mathrm{L}}}} \eta_{p_1}(p_1+u_1-u_2)^2\eta_{p_1+u_1-u_2}\,\mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0]. \tag{3.35}$$

The function $\gamma(p)$ is defined in (2.21).

Proof. It is convenient to introduce the operators

$$\mathcal{K}_{\mathrm{B}} = \sum_{p\in P_{\mathrm{B}}} p^2a^*_pa_p, \qquad \mathcal{K}_{\mathrm{I}} = \sum_{p\in P_{\mathrm{I}}} p^2a^*_pa_p \qquad \text{and} \qquad \mathcal{K}_{>} = \sum_{p\in P^c_{\mathrm{L}}} p^2a^*_pa_p \tag{3.36}$$

and to denote the corresponding expectations w.r.t. Γ by $\mathcal{G}_{\mathcal{K}_{\mathrm{B}}}, \mathcal{G}_{\mathcal{K}_{\mathrm{I}}}, \mathcal{G}_{\mathcal{K}_{>}}$, i.e.,

$$\mathcal{G}_{\mathcal{K}} = \sum_{\alpha} \lambda_\alpha \frac{\langle (1+B)\psi_\alpha, (\mathcal{K}_{\mathrm{B}} + \mathcal{K}_{\mathrm{I}} + \mathcal{K}_{>})(1+B)\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle} = \mathcal{G}_{\mathcal{K}_{\mathrm{B}}} + \mathcal{G}_{\mathcal{K}_{\mathrm{I}}} + \mathcal{G}_{\mathcal{K}_{>}}. \tag{3.37}$$

In the next subsections we will prove upper bounds for $\mathcal{G}_{\mathcal{K}_{\mathrm{B}}}, \mathcal{G}_{\mathcal{K}_{\mathrm{I}}}$ and $\mathcal{G}_{\mathcal{K}_{>}}$. We will need to compute the commutators of $\mathcal{K}_{\mathrm{I}}$ and $\mathcal{K}_{>}$ with B. Indicating with $P_{\#}$ either P_{I} or $P_{\mathrm{L}}^{\mathrm{c}}$ and with $\mathcal{K}_{\#}$ either $\mathcal{K}_{\mathrm{I}}$ or $\mathcal{K}_{>}$, we will use the result

$$\begin{aligned} [\mathcal{K}_{\#}, B] &= \frac{1}{2|\Lambda|} \sum_{\substack{q\in P_{\#}, p\in P_{\mathrm{H}},\\ u,v\in P_{\mathrm{L}}}} q^2 \eta_p [a_q^* a_q, a_{u+p}^* a_{v-p}^* a_u a_v] \\ &= \frac{1}{|\Lambda|} \sum_{\substack{q\in P_{\#}, p\in P_{\mathrm{H}},\\ u,v\in P_{\mathrm{L}}}} q^2 \eta_p \left(\delta_{q,u+p} a_q^* a_{v-p}^* a_u a_v - \delta_{q,u}\, a_{u+p}^* a_{v-p}^* a_v a_q\right), \end{aligned} \tag{3.38}$$

where we exploited the symmetry $\eta_p = \eta_{-p}$.

3.2.1. Analysis of $\mathcal{G}_{\mathcal{K}_{\mathrm{B}}}$

Using the positivity of $\mathcal{K}_{\mathrm{B}}$ we estimate the denominator by one; observing that $\langle \psi_\alpha, (B^* \mathcal{K}_{\mathrm{B}} + \mathcal{K}_{\mathrm{B}} B)\, \psi_\alpha\rangle$ vanishes (because the creation operators in B commute with $\mathcal{K}_{\mathrm{B}}$ and give zero when acting on ψ_α), we have

$$\begin{aligned} \mathcal{G}_{\mathcal{K}_{\mathrm{B}}} &= \sum_{\alpha} \lambda_\alpha \frac{\langle (1+B)\psi_\alpha, \mathcal{K}_{\mathrm{B}}(1+B)\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle} \le \sum_{\alpha} \lambda_\alpha \, \langle \psi_\alpha, \Big(\sum_{p\in P_{\mathrm{B}}} p^2 a_p^* a_p\Big)\psi_\alpha\rangle + \sum_{\alpha} \lambda_\alpha \, \langle \psi_\alpha, B^* \mathcal{K}_{\mathrm{B}} B\, \psi_\alpha\rangle \\ &= \sum_{p\in P_{\mathrm{B}}} p^2 \gamma(p) + \mathcal{E}_{\mathcal{K}_{\mathrm{B}}}. \end{aligned} \tag{3.39}$$

To estimate the error term in (3.39) we contract the annihilation operators with momenta in P_{H} in B^* with those in B, and obtain

$$\begin{aligned} |\mathcal{E}_{\mathcal{K}_{\mathrm{B}}}| &= \frac{1}{2|\Lambda|^2} \Bigg| \sum_{\substack{p_1\in P_{\mathrm{H}}, q\in P_{\mathrm{B}}\\ u_1,v_1,u_2\in P_{\mathrm{L}}}} q^2\, \eta_{p_1}\, \eta_{p_1+u_1-u_2}\, \mathrm{Tr}[a_{u_1}^* a_{v_1}^* a_q^* a_q a_{u_2} a_{u_1+v_1-u_2} \Gamma_0] \Bigg| \\ &\lesssim \frac{N^{-3+\delta_{\mathrm{H}}+2\delta_{\mathrm{B}}}}{L^2} \sum_{\substack{q\in P_{\mathrm{B}}\\ u_1,v_1,u_2\in P_{\mathrm{L}}}} \Big| \mathrm{Tr}[a_{u_1}^* a_{v_1}^* a_q^* a_q a_{u_2} a_{u_1+v_1-u_2} \Gamma_0] \Big| \lesssim L^{-2} N^{\delta_{\mathrm{H}}+2\delta_{\mathrm{B}}}. \end{aligned} \tag{3.40}$$

The inequalities follow from $|q| \le N^{\delta_{\mathrm{B}}}$, the Cauchy-Schwarz inequality, the bound in (A.8) and Lemma 2.8. We therefore have

$$\mathcal{G}_{\mathcal{K}_{\mathrm{B}}} - \sum_{p\in P_{\mathrm{B}}} p^2 \gamma(p) \lesssim L^{-2} N^{\delta_{\mathrm{H}}+2\delta_{\mathrm{B}}}. \tag{3.41}$$

3.2.2. Analysis of $\mathcal{G}_{\mathcal{K}_{\mathrm{I}}}$

Here we need to exploit crucial cancellations between the numerator and the denominator. We commute $\mathcal{K}_{\mathrm{I}}$ to the right and obtain

$$\mathcal{G}_{\mathcal{K}_{\mathrm{I}}} = \sum_{\alpha} \lambda_\alpha \frac{\langle (1+B)\psi_\alpha, \mathcal{K}_{\mathrm{I}}(1+B)\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle} = \sum_{\alpha} \lambda_\alpha \frac{\langle (1+B)\psi_\alpha, (1+B)\mathcal{K}_{\mathrm{I}}\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle} + \mathcal{E}_{\mathcal{G}_{\mathcal{K}_{\mathrm{I}}}}$$

with

$$\mathcal{E}_{\mathcal{G}_{K_\mathrm{I}}} := \sum_\alpha \lambda_\alpha \frac{\langle \psi_\alpha, (1+B^*)[\mathcal{K}_\mathrm{I}, B]\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle}. \tag{3.42}$$

Let us introduce the notation $\psi_\alpha = \xi_{\alpha_1} \otimes \nu_{\alpha_2}$ with $\alpha = (\alpha_1, \alpha_2)$, where ξ_{α_1} and ν_{α_2} denote the eigenfunctions of G_B and G_free, respectively. Calling E_{α_2} the eigenvalues of $\mathcal{K}_\mathrm{I}$, so that $\mathcal{K}_\mathrm{I}\nu_{\alpha_2} = E_{\alpha_2}\nu_{\alpha_2}$, we see that

$$\mathcal{G}_{\mathcal{K}_\mathrm{I}} = \sum_\alpha \lambda_\alpha E_{\alpha_2} + \mathcal{E}_{\mathcal{G}_{K_\mathrm{I}}} \tag{3.43}$$

holds.

Next, we estimate $\mathcal{E}_{\mathcal{G}_{K_\mathrm{I}}}$. With $\|(1+B)\psi_\alpha\| \geq 1$ we have

$$|\mathcal{E}_{\mathcal{G}_{K_\mathrm{I}}}| = \left| \sum_\alpha \lambda_\alpha \frac{\langle \psi_\alpha, B^*[\mathcal{K}_\mathrm{I}, B]\psi_\alpha\rangle}{\langle (1+B)\psi_\alpha, (1+B)\psi_\alpha\rangle} \right| \leq \sum_\alpha \lambda_\alpha |\langle \psi_\alpha, B^*[\mathcal{K}_\mathrm{I}, B]\psi_\alpha\rangle|. \tag{3.44}$$

When we contract the high momenta in $B^*[\mathcal{K}_\mathrm{I}, B]$, we see that the inner product inside the absolute value equals

$$\langle \psi_\alpha, B^*[\mathcal{K}_\mathrm{I}, B]\psi_\alpha\rangle = -\frac{1}{|\Lambda|^2} \sum_{\substack{u_1, v_1 \in P_\mathrm{L} \\ p_1 \in P_\mathrm{H},\, u_2 \in P_\mathrm{I}}} u_2^2\, \eta_{p_1+v_1-u_2} \eta_{p_1} \langle \psi_\alpha,\, a^*_{u_1} a^*_{v_1} a_{u_2} a_{u_1+v_1-u_2} \psi_\alpha\rangle\,. \tag{3.45}$$

Applying the Cauchy-Schwarz inequality, using (A.8), and estimating $|u_2| \leq N^{1/3+\delta_\mathrm{L}}/L$ we find

$$\begin{aligned}\sum_\alpha \lambda_\alpha |\langle \psi_\alpha, B^*[\mathcal{K}_\mathrm{I}, B]\psi_\alpha\rangle| &\leq \frac{1}{|\Lambda|^2} \sum_\alpha \lambda_\alpha \sum_{\substack{u_1, v_1 \in P_\mathrm{L} \\ u_2 \in P_\mathrm{I}}} |\langle \psi_\alpha, a^*_{u_1} a^*_{v_1} a_{u_2} a_{u_1+v_1-u_2}\psi_\alpha\rangle| \sum_{p_1 \in P_\mathrm{H}} |\eta_{p_1+u_1-u_2}\eta_{p_1}\, u_2^2| \\ &\lesssim L^{-2} N^{-7/3+\delta_\mathrm{H}+2\delta_\mathrm{L}} \sum_\alpha \lambda_\alpha \sum_{\substack{u_1, v_1 \in P_\mathrm{L} \\ u_2 \in P_\mathrm{I}}} |\langle \psi_\alpha, a^*_{u_1} a^*_{v_1} a_{u_2} a_{u_1-v_1+u_2}\psi_\alpha\rangle|. \end{aligned} \tag{3.46}$$

We observe now that since $u_2 \in P_\mathrm{I}$, at least one of the momenta u_1 or v_1 needs to be in P_I (this is due to the fact that the eigenfunctions of G_free are symmetric tensor products of plane waves). Let us assume without loss of generality that $v_1 \in P_\mathrm{I}$. We distinguish now the three cases $u_1 = 0$, $u_1 \in P_\mathrm{B}$ and $u_1 \in P_\mathrm{I}$.

If $u_1 = 0$, then $v_1 - u_2 = 0$ (this again follows from the structure of the orthonormal set $\{\psi_\alpha\}_{\alpha \in \mathbb{N}}$), and the expectation $\langle \psi_\alpha, a_0^* a_{u_2}^* a_{u_2} a_0 \psi_\alpha\rangle$ is positive. In this case we estimate the sum on the r.h.s. (3.46) by

$$\begin{aligned}\sum_\alpha \lambda_\alpha \sum_{u_2 \in P_\mathrm{I}} \langle \psi_\alpha, a_0^* a_{u_2}^* a_{u_2} a_0 \psi_\alpha\rangle &= \sum_{u_2 \in P_\mathrm{I}} \mathrm{Tr}\,[a_0^* a_{u_2}^* a_{u_2} a_0\, \Gamma_0] \\ &= \int_\mathbb{C} \mathrm{Tr}_{\mathscr{F}_0}\,[a_0^* a_0\, |z\rangle\langle z|]\zeta(z)\,\mathrm{d}z\ \ \mathrm{Tr}_{\mathscr{F}_\mathrm{I}}\Big[\sum_{u_2 \in P_\mathrm{I}} a^*_{u_2} a_{u_2}\, \Gamma_\mathrm{free}\Big] = \int_\mathbb{C} |z|^2 \zeta(z)\,\mathrm{d}z \sum_{u_2 \in P_\mathrm{I}} \gamma(u_2) \leq N^2. \end{aligned} \tag{3.47}$$

To obtain the last inequality we used $\widetilde{N}_0 + \sum_{p \in \Lambda_+^*} \gamma(p) = N$.

In the case $u_1 \in P_\mathrm{B}$ we have $v_1 = u_2$ and $u_1 - v_1 + u_2 = u_1$ because G_B and G_free are both translation-invariant states. In particular, the relevant expectation value is again positive. Using (2.28) we obtain the following bound for the sum on the r.h.s. of (3.46):

$$\begin{aligned}\sum_\alpha \lambda_\alpha \sum_{\substack{u_1 \in P_\mathrm{B} \\ v_1, u_2 \in P_\mathrm{I}}} |\langle \psi_\alpha, a^*_{u_1} a^*_{v_1} a_{u_2} a_{u_1-v_1+u_2} \psi_\alpha\rangle| &= \sum_\alpha \lambda_\alpha \sum_{\substack{u_1 \in P_\mathrm{B} \\ u_2 \in P_\mathrm{I}}} \langle \psi_\alpha, a^*_{u_2} a_{u_2} a^*_{u_1} a_{u_1} \psi_\alpha\rangle \\ &= \int_\mathbb{C} \mathrm{Tr}_{\mathscr{F}_\mathrm{B}}\Big[\sum_{u_1 \in P_\mathrm{B}} a^*_{u_1} a_{u_1}\, G_\mathrm{B}(z)\Big]\zeta(z)\,\mathrm{d}z\ \ \mathrm{Tr}_{\mathscr{F}_\mathrm{I}}\Big[\sum_{u_2 \in P_\mathrm{I}} a^*_{u_2} a_{u_2}\, G_\mathrm{free}\Big] \lesssim N^{5/3+\delta_\mathrm{B}} \end{aligned} \tag{3.48}$$

To conclude the discussion, we examine the case $u_1 \in P_{\mathrm{I}}$. This implies that $u_1 - v_1 + u_2 \in P_{\mathrm{I}}$. Moreover, we have that either $v_1 = u_2$ or $u_1 = u_2$; in both cases the expectation is positive. An application of Lemma 2.8 shows

$$\sum_\alpha \lambda_\alpha \sum_{u_1,u_2\in P_{\mathrm{I}}} \langle \psi_\alpha, a^*_{u_1} a^*_{u_2} a_{u_2} a_{u_1} \psi_\alpha\rangle = \sum_{u_1,u_2\in P_{\mathrm{I}}} \operatorname{Tr}_{\mathscr{F}_{\mathrm{I}}} \left[a^*_{u_1} a^*_{u_2} a_{u_2} a_{u_1} \Gamma_0 \right] \lesssim N^2 \tag{3.49}$$

as a bound for the sum on the r.h.s. of (3.46).

In combination, (3.44), (3.46)–(3.49), and $\delta_{\mathrm{B}} < 1/3$ imply

$$|\mathcal{E}_{\mathcal{G}_{K_{\mathrm{I}}}}| \lesssim L^{-2} N^{-1/3+\delta_{\mathrm{H}}+2\delta_L} \tag{3.50}$$

as well as

$$\Big|\mathcal{G}_{\mathcal{K}_{\mathrm{I}}} - \sum_\alpha \lambda_\alpha E_{\alpha_2}\Big| = \Big|\mathcal{G}_{\mathcal{K}_{\mathrm{I}}} - \sum_{p\in P_{\mathrm{I}}} p^2 \gamma(p)\Big| \lesssim L^{-2} N^{-1/3+\delta_{\mathrm{H}}+2\delta_L}. \tag{3.51}$$

To obtain (3.51), we additionally used (3.43) and Lemma 2.3.

3.2.3. Analysis of $\mathcal{G}_{\mathcal{K}_>}$

In the analysis of $\mathcal{G}_{\mathcal{K}_>}$ we estimate the denominator again by one. When we additionally commute $\mathcal{K}_>$ to the right we find

$$\begin{aligned} \mathcal{G}_{\mathcal{K}_>} &\leq \sum_\alpha \lambda_\alpha \langle (1+B)\psi_\alpha, \mathcal{K}_> (1+B)\psi_\alpha \rangle \\ &= \sum_\alpha \lambda_\alpha \langle (1+B)\psi_\alpha, (1+B)\mathcal{K}_> \psi_\alpha \rangle + \sum_\alpha \lambda_\alpha \langle \psi_\alpha, (1+B^*)[\mathcal{K}_>, B]\psi_\alpha \rangle . \end{aligned} \tag{3.52}$$

The first contribution clearly vanishes because it contains annihilation operators with momenta in $P_{\mathrm{L}}^{\mathrm{c}}$ acting on ψ_α. Using additionally (3.38), we see that

$$[\mathcal{K}_>, B] = \frac{1}{|\Lambda|} \sum_{\substack{p\in P_{\mathrm{H}}\\ u,v\in P_{\mathrm{L}}}} p^2 \eta_p \, a^*_{u+p} a^*_{v-p} a_u a_v + \frac{2}{|\Lambda|} \sum_{\substack{p\in P_{\mathrm{H}}\\ u,v\in P_{\mathrm{L}}}} \eta_p \, u\cdot p \, a^*_{u+p} a^*_{v-p} a_u a_v =: \mathcal{K}_\eta + \mathcal{E}_{\mathcal{K}}, \tag{3.53}$$

which implies

$$\mathcal{G}_{\mathcal{K}_>} \leq \sum_\alpha \lambda_\alpha \langle \psi_\alpha, (1+B^*)(\mathcal{K}_\eta + \mathcal{E}_{\mathcal{K}})\psi_\alpha\rangle = \operatorname{Tr}[B^* \mathcal{K}_\eta \Gamma_0] + \operatorname{Tr}[B^* \mathcal{E}_{\mathcal{K}} \Gamma_0]. \tag{3.54}$$

When we contract operators with high momenta this allows us to write the first term on the r.h.s. as

$$\begin{aligned} \operatorname{Tr}[B^* \mathcal{K}_\eta \Gamma_0] &= \frac{1}{|\Lambda|^2} \sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1\in P_{\mathrm{L}}}} \eta_{p_1} \sum_{\substack{p_2\in P_{\mathrm{H}}\\ u_2,v_2\in P_{\mathrm{L}}}} p_2^2 \eta_{p_2} \operatorname{Tr}[a^*_{v_1} a^*_{u_1} a_{v_2} a_{u_2} \Gamma_0] \delta_{u_2+p_2,u_1+p_1} \delta_{v_2-p_2,v_1-p_1} \\ &= \frac{1}{|\Lambda|^2} \sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2,v_2\in P_{\mathrm{L}}}} \eta_{p_1} (p_1+u_1-u_2)^2 \eta_{p_1+u_1-u_2} \operatorname{Tr}[a^*_{v_1} a^*_{u_1} a_{v_2} a_{u_2} \Gamma_0] \delta_{v_2, v_1+u_1-u_2}. \end{aligned} \tag{3.55}$$

Because Γ_0 is translation invariant the factor $\delta_{v_2,v_1+u_1-u_2}$ can be dropped. This term contributes to (3.35).

We consider now the second term in (3.54), that is,

$$\operatorname{Tr}[B^* \mathcal{E}_{\mathcal{K}} \Gamma_0] = \frac{2}{|\Lambda|^2} \sum_{u_1,v_1\in P_{\mathrm{L}}} \sum_{\substack{p_2\in P_{\mathrm{H}}\\ u_2,v_2\in P_{\mathrm{L}}}} \eta_{p_2+u_2-u_1} \eta_{p_2} p_2 \cdot u_2 \operatorname{Tr}[a^*_{v_1} a^*_{u_1} a_{v_2} a_{u_2} \Gamma_0]. \tag{3.56}$$

An application of Lemma 2.7 shows that the trace in (3.56) can be written as $\mathrm{Tr}[B^*\mathcal{E}_{\mathcal{K}}\,\Gamma_0] = \mathrm{D}_1 + \mathrm{D}_2$ with

$$\mathrm{D}_1 = 2\widetilde{N}_0|\Lambda|^{-2} \sum_{p_2\in P_{\mathrm{H}},u_2\in P_{\mathrm{L}}} \Big[(\eta_{p_2} + \eta_{p_2+u_2})\eta_{p_2} p_2\cdot u_2\,\gamma(u_2) + \eta_{p_2+u_2}\eta_{p_2} p_2\cdot u_2\,\alpha(u_2)\Big],$$
$$\mathrm{D}_2 = 2|\Lambda|^{-2} \sum_{\substack{p_2\in P_{\mathrm{H}}\\ v_2,u_2\in P_{\mathrm{L}}}} \Big[(\eta_{p_2} + \eta_{p_2-v_2+u_2})\eta_{p_2} p_2\cdot u_2\,\gamma(u_2)\gamma(v_2) + \eta_{p_2-v_2+u_2}\eta_{p_2} p_2\cdot u_2\,\overline{\alpha(v_2)}\alpha(u_2)\Big]. \tag{3.57}$$

Let us introduce the set $P_r := \{p\in\Lambda^* : |p|\geq rN\}$, where $r>1$; for $p_2\in P_r$ we have

$$\sup_{u\in P_{\mathrm{L}}} \sum_{p_2\in P_r} |\eta_{p_2-u}\eta_{p_2}||p_2| \leq \Big(\sum_{p\in P_{r/2}} |\eta_p|^2\Big)^{1/2}\Big(\sum_{q\in P_r} |\eta_q|^2 q^2\Big)^{1/2} \lesssim_r L^5 N^{-2}, \tag{3.58}$$

which follows from the Cauchy-Schwarz inequality, (A.7) and (A.4) (the latter implies $\|\nabla f_N\|_{L^2}\lesssim L^2N^{-1/2}$). Instead, for $p_2\in P_r^{\mathrm{c}}$, (A.7) implies

$$\sup_{u\in P_{\mathrm{L}}} \sum_{p_2\in P_{\mathrm{H}}\cap P_r^{\mathrm{c}}} |\eta_{p_2}\eta_{p_2-u}||p_2| \lesssim \frac{L^2}{N^2}\sup_{u\in P_{\mathrm{L}}} \sum_{p_2\in P_{\mathrm{H}}\cap P_r^{\mathrm{c}}} \frac{1}{|p_2|(|p_2|-|u|)^2} \lesssim \frac{L^5\ln(N)}{N^2}. \tag{3.59}$$

To obtain the second bound we used $|p_2|-|u|\gtrsim 1$, which follows from the assumption $\delta_{\mathrm{L}}+\delta_{\mathrm{H}}<2/3$. Using (2.27), (3.58), (3.59) and $\delta_{\mathrm{B}}<1/3$, we conclude that

$$\begin{aligned}|\mathrm{D}_1| &\lesssim (\widetilde{N}_0/|\Lambda|^2)\sup_{u\in P_{\mathrm{L}}}\sum_{p_2\in P_{\mathrm{H}}}|\eta_{p_2-u}\eta_{p_2}||p_2|\sum_{u_2\in P_{\mathrm{L}}}|u_2|\gamma(u_2) + (\widetilde{N}_0/|\Lambda|^2)\sup_{u\in P_{\mathrm{L}}}\sum_{p_2\in P_{\mathrm{H}}}|\eta_{p_2-u}\eta_{p_2}||p_2|\sum_{u_2\in P_{\mathrm{L}}}|u_2||\alpha(u_2)|\\ &\lesssim L^{-2}N^{1/3}\ln(N).\end{aligned} \tag{3.60}$$

With similar considerations we see that

$$\begin{aligned}|\mathrm{D}_2| \lesssim& \frac{1}{|\Lambda|^2}\sup_{u\in P_{\mathrm{L}}}\sum_{p_2\in P_{\mathrm{H}}}|\eta_{p_2-u}\eta_{p_2}||p_2|\sum_{u_2,v_2\in P_{\mathrm{L}}}|u_2|\gamma(u_2)\gamma(v_2)\\ &+\frac{1}{|\Lambda|^2}\sup_{u\in P_{\mathrm{L}}}\sum_{p_2\in P_{\mathrm{H}}}|\eta_{p_2-u}\eta_{p_2}||p_2|\sum_{u_2,v_2\in P_{\mathrm{L}}}|u_2||\alpha(u_2)\alpha(v_2)| \lesssim L^{-2}N^{1/3}\ln(N).\end{aligned} \tag{3.61}$$

Collecting the results of equations (3.54)–(3.56) and the bounds (3.60), (3.61), we conclude that

$$\mathcal{G}_{\mathcal{K}_>} - \frac{1}{|\Lambda|^2}\sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2,v_2\in P_{\mathrm{L}}}} \eta_{p_1}(p_1+u_1-u_2)^2\eta_{p_1+u_1-u_2}\ \mathrm{Tr}[a^*_{v_1}a^*_{u_1}a_{v_2}a_{u_2}\Gamma_0] \lesssim L^{-2}N^{1/3}\ln(N). \tag{3.62}$$

The bounds (3.41), (3.51) and (3.62) imply (3.35) and conclude the proof of Lemma 3.4. □

3.3. Proof of Proposition 3.1

The results of Lemma 3.3 and Lemma 3.4 imply

$$\mathrm{Tr}\,[\mathcal{H}_N\Gamma] - (E_{\mathcal{K}} + E_{\mathcal{V}_N}) \lesssim L^{-2}\mathcal{E}_N, \tag{3.63}$$

with $E_{\mathcal{V}_N}$ in (3.7), $E_{\mathcal{K}}$ in (3.35) and

$$\mathcal{E}_N = N^{1-\delta_{\mathrm{H}}} + N^{\delta_{\mathrm{H}}+2\delta_{\mathrm{B}}} + N^{-1/3+\delta_{\mathrm{H}}+2\delta_L} + N^{1/3}\ln(N). \tag{3.64}$$

Separating the contributions from momenta in P_{B} and P_{I}, $E_{\mathcal{V}_N} + E_{\mathcal{K}}$ can be written as

$$E_{\mathcal{K}} + E_{\mathcal{V}_N} = \mathrm{Tr}_{\mathscr{F}_{\mathrm{I}}}\Big[\Big(\sum_{p\in P_{\mathrm{I}}} p^2 a_p^* a_p\Big) G_{\mathrm{free}}\Big] + \frac{\widetilde{N}_0}{|\Lambda|}\sum_{q\in P_{\mathrm{I}}} (\hat{v}_N * \hat{f}_N)(q)\gamma(q)$$
$$+ \mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}}\Big[\sum_{p\in P_{\mathrm{B}}} p^2 a_p^* a_p + \frac{\widetilde{N}_0}{2|\Lambda|}\sum_{q\in P_{\mathrm{B}}}(\hat{v}_N * \hat{f}_N)(q)\Big(2a_q^*a_q + (z/|z|)^2 a_q^* a_{-q}^* + (\bar{z}/|z|)^2 a_q a_{-q}\Big) G_{\mathrm{B}}(z)\Big]$$
$$+ \frac{4\pi\mathfrak{a}}{N|\Lambda|}\Big[\int_{\mathbb{C}} |z|^4 \zeta(z)\,\mathrm{d}z + 2\widetilde{N}_0 \sum_{u\in P_{\mathrm{L}}\backslash\{0\}} \gamma(u) + 2\sum_{u,v\in P_{\mathrm{L}}\backslash\{0\}} \gamma(v)\gamma(u)\Big] + \mathrm{E}_1 \tag{3.65}$$

with

$$\mathrm{E}_1 = \frac{1}{|\Lambda|^2}\sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2\in P_{\mathrm{L}}}} \eta_{p_1}\Big[(p_1+u_1-u_2)^2\eta_{p_1+u_1-u_2} + \frac{1}{2}\hat{v}_N(p_1+u_1-u_2)$$
$$+ \frac{1}{2|\Lambda|}\sum_{p_2\in P_{\mathrm{H}}} \hat{v}_N(p_1+p_2+u_1-u_2)\eta_{p_2}\Big]\,\mathrm{Tr}[a_{v_1}^* a_{u_1}^* a_{v_2} a_{u_2}\Gamma_0]. \tag{3.66}$$

An application of the scattering equation in (A.6) allows us to write E_1 as

$$\mathrm{E}_1 = \frac{1}{|\Lambda|}\sum_{\substack{p_1\in P_{\mathrm{H}}\\ u_1,v_1,u_2\in P_{\mathrm{L}}}} \eta_{p_1}\Big[\lambda_N(\hat{\mathbb{1}}_{|x|\le \ell} * \hat{f}_N)(p_1+u_1-u_2) - \frac{1}{2|\Lambda|}\sum_{p_2\in P_{\mathrm{H}}^c} \hat{v}_N(p_1+p_2+u_1-u_2)\eta_{p_2}\Big]\mathrm{Tr}[a_{v_1}^* a_{u_1}^* a_{v_2} a_{u_2}\Gamma_0]$$
$$=: \mathrm{E}_{11} + \mathrm{E}_{12}. \tag{3.67}$$

We now prove

$$|\mathrm{E}_{11}| \lesssim L^{-2}N^{-1/2+\delta_{\mathrm{H}}/2} \quad \text{and} \quad |\mathrm{E}_{12}| \lesssim L^{-2}N^{1-\delta_{\mathrm{H}}}. \tag{3.68}$$

To obtain the bound for E_{11}, we first note that (A.4) and $f_N \le 1$ imply

$$\sum_{p_1\in\Lambda^*} |(\hat{\mathbb{1}}_{|x|\le\ell} * \hat{f}_N)(p_1)|^2 = \|\mathbb{1}_{|x|\le\ell} f_N\|^2 \lesssim L^3 N^{-2}. \tag{3.69}$$

Applications of the above bound, Cauchy-Schwarz, (A.2) (which implies $\lambda_N \lesssim 1/(NL^2)$), (A.8) and Lemma 2.8 prove the bound for E_{11}. An application of (A.7) shows

$$\sup_{u\in\Lambda^*}\sum_{p\in P_{\mathrm{H}}} |\hat{v}_N(p+u)||\eta_p| \le \frac{L\|\hat{v}\|_\infty}{N^2}\sum_{\substack{p\in P_{\mathrm{H}},\\ |p|\le N}} \frac{1}{p^2} + \Big(\sum_{p\in\Lambda^*}|\hat{v}_N(p)|^2\Big)^{1/2}\Big(\sum_{|p|>N}\frac{L^2}{N^2p^4}\Big)^{1/2} \lesssim L^4N^{-1}. \tag{3.70}$$

The bound for E_{12} follows when we combine this bound, (A.9) and Lemma 2.8.

Next, we use (2.27) and (3.18) to estimate

$$\frac{\widetilde{N}_0}{|\Lambda|}\sum_{q\in P_{\mathrm{I}}}(\hat{v}_N * \hat{f}_N)(q)\gamma(q) \le \frac{8\pi\mathfrak{a}\widetilde{N}_0}{N|\Lambda|}\sum_{q\in P_{\mathrm{I}}}\gamma(q) + CL^{-2}. \tag{3.71}$$

Finally, we can replace $\widetilde{N}_0$ by $N_0(\beta,N,L)$ in the second line of (3.65). More precisely, we apply Lemmas 2.5, 2.6 and (3.18) and find that the error term is bounded by

$$\frac{|\widetilde{N}_0 - N_0|}{|\Lambda|}\sum_{q\in P_{\mathrm{B}}}\Big|(\hat{v}_N * \hat{f}_N)(q)\Big|(2\gamma(q) + |\alpha(q)| + |\overline{\alpha(q)}|) \lesssim L^{-2}N^{1/3+\delta_{\mathrm{B}}}. \tag{3.72}$$

In combination, (3.63), (3.65)–(3.68), (3.71) and (3.72) prove (3.1).

4. Bound for the entropy

In this section we establish the following lower bound for the entropy of our trial state.

Proposition 4.1. *There exists a constant $C > 0$ such that the entropy of the state Γ in (2.13) satisfies*

$$S(\Gamma) \geq \int_{\mathbb{C}} S(G_{\mathrm{B}}(z))\zeta(z)\,\mathrm{d}z + S(G_{\mathrm{free}}) + S(\zeta) - CN^{-1+\delta_{\mathrm{H}}}, \tag{4.1}$$

where

$$S(\zeta) = -\int_{\mathbb{C}} \zeta(z)\ln(\zeta(z))\,\mathrm{d}z \tag{4.2}$$

denotes the classical entropy of the probability distribution ζ.

The remainder of this section is devoted to the proof of Proposition 4.1. In the first step, we estimate the influence of the correlation structure with the following lemma. It appeared for the first time in [57, Lemma 2].

Lemma 4.2. *Let Γ be a density matrix on some Hilbert space with eigenvalues $\{\lambda_\alpha\}_{\alpha\in\mathbb{N}}$, let $\{P_\alpha\}_{\alpha\in\mathbb{N}}$ be a family of one-dimensional orthogonal projection (for which $P_{\alpha_1}P_{\alpha_2} = \delta_{\alpha_1,\alpha_2}P_{\alpha_1}$ need not necessarily be true), and define $\hat{\Gamma} = \sum_\alpha \lambda_\alpha P_\alpha$. Then we have*

$$S(\hat{\Gamma}) \geq S(\Gamma) - \ln \operatorname{Tr}\left(\sum_\alpha P_\alpha \hat{\Gamma}\right). \tag{4.3}$$

An application of Lemma 4.2 shows

$$S(\Gamma) \geq S(\Gamma_0) - \ln \operatorname{Tr}\left(\sum_{\alpha'} |\phi_{\alpha'}\rangle\langle\phi_{\alpha'}|\,\Gamma\right) = S(\Gamma_0) - \ln\left(\sum_{\alpha,\alpha'} \lambda_\alpha\, |\langle\phi_\alpha,\phi_{\alpha'}\rangle|^2\right) \tag{4.4}$$

with Γ_0 in (2.7) and λ_α, ϕ_α in (2.13). Let us have a closer look at the term inside the logarithm. Using $\|(1+B)\psi_\alpha\| \geq 1$, $B^*\psi_\alpha = 0$ and the fact that $\{\psi_\alpha\}_{\alpha\in\mathbb{N}}$ is an orthonormal set, we see that

$$\begin{aligned}\sum_{\alpha,\alpha'} \lambda_\alpha\, |\langle\phi_\alpha,\phi_{\alpha'}\rangle|^2 &\leq \sum_{\alpha,\alpha'} \lambda_\alpha\, |\langle\psi_\alpha,(1+B^*)(1+B)\psi_{\alpha'}\rangle|^2 = 1 + 2\sum_\alpha \lambda_\alpha\langle\psi_\alpha, B^*B\psi_\alpha\rangle + \sum_\alpha \lambda_\alpha\langle\psi_\alpha,(B^*B)^2\psi_\alpha\rangle \\ &\leq 1 + \delta + (1+\delta^{-1})\operatorname{Tr}\left[(B^*B)^2\Gamma_0\right] \end{aligned}\tag{4.5}$$

holds for $\delta > 0$.

The last term on the r.h.s. reads

$$\begin{aligned}\operatorname{Tr}\left[(B^*B)^2\Gamma_0\right] = \frac{1}{16|\Lambda|^4} &\sum_{p_i\in P_{\mathrm{H}};u_i,v_i\in P_{\mathrm{L}}} \prod_{i=1}^4 \eta_{p_i} \\ &\times \operatorname{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_1+p_1}a_{v_1-p_1}a^*_{u_2+p_2}a^*_{v_2-p_2}a_{u_2}a_{v_2}a^*_{u_3}a^*_{v_3}a_{u_3+p_3}a_{v_3-p_3}a^*_{u_4+p_4}a^*_{v_4-p_4}a_{u_4}a_{v_4}\Gamma_0\right].\end{aligned} \tag{4.6}$$

Since no momenta in $P_{\mathrm{H}} - P_{\mathrm{L}}$ are present in the state Γ_0, we know that the operators with momenta in $P_{\mathrm{H}} - P_{\mathrm{L}}$ need to be paired among each other in order to obtain a non-zero contribution. A short computation therefore shows that the r.h.s. of (4.6) is bounded from above by a constant times

$$\frac{1}{|\Lambda|^4}\left(\sum_{p,q\in P_{\mathrm{H}}+P_{\mathrm{L}}} |\eta_p\eta_q|\right)^2 \sum_{u_i,v_i\in P_{\mathrm{L}}} \operatorname{Tr}\left[a^*_{u_1}a^*_{v_1}a_{u_2}a_{v_2}a^*_{u_3}a^*_{v_3}a_{u_4}a_{v_4}\Gamma_0\right]. \tag{4.7}$$

We apply the Cauchy-Schwarz inequality and (A.8) to bound the proportional to $\eta_p \eta_q$ by $\sum_{p \in P_{\mathrm{H}}+P_{\mathrm{L}}} \eta_p^2 \lesssim L^6 N^{-3+\delta_{\mathrm{H}}}$. Afterwards, we use Lemma 2.8 to show that the second factor is bounded by a constant times N^4. When we put the above considerations together together, use $\delta_{\mathrm{L}} + \delta_{\mathrm{H}} < 2/3$, and choose $\delta = N^{-1+\delta_{\mathrm{H}}}$, we find

$$\sum_{\alpha,\alpha'} \lambda_\alpha \, |\langle \phi_\alpha, \phi_{\alpha'} \rangle|^2 \leq 1 + CN^{-1+\delta_{\mathrm{H}}} \tag{4.8}$$

as well as

$$S(\Gamma) \geq S(\Gamma_0) - CN^{-1+\delta_{\mathrm{H}}}. \tag{4.9}$$

It remains to find a lower bound for the entropy of Γ_0.

To that end, we need the following lemma, which provides us with a Berezin–Lieb inequality in the spirit of [9, 38].

Lemma 4.3. *Let $\{G(z)\}_{z\in\mathbb{C}}$ be a family of states on a Hilbert space, let $p : \mathbb{C} \to \mathbb{R}$ be a probability distribution and define the state*

$$\Gamma = \int_{\mathbb{C}} |z\rangle\langle z| \otimes G(z) p(z) \, \mathrm{d}z. \tag{4.10}$$

Then we have

$$S(\Gamma) \geq \int_{\mathbb{C}} S(G(z)) p(z) \, \mathrm{d}z + S(p) \quad \textit{with} \quad S(p) = -\int_{\mathbb{C}} p(z) \ln(p(z)) \, \mathrm{d}z. \tag{4.11}$$

Proof. We use the spectral theorem to write

$$G(z) = \sum_\alpha g_\alpha(z) \, |v_\alpha(z)\rangle\langle v_\alpha(z)| \quad \text{as well as} \quad |z\rangle\langle z| \otimes G(z) = \sum_\alpha g_\alpha(z) \, |z \otimes v_\alpha(z)\rangle\langle z \otimes v_\alpha(z)|. \tag{4.12}$$

Because $G(z)$ is a state for fixed $z \in \mathbb{C}$, we know that $\{v_\alpha(z)\}_{\alpha\in\mathbb{N}}$ is an orthonormal basis. In combination with the completeness relation $\int |z\rangle\langle z| \, \mathrm{d}z = \mathbb{1}$, this implies

$$\int_{\mathbb{C}} \sum_{\alpha=1}^{\infty} |\langle w, z \otimes v_\alpha(z) \rangle|^2 \, \mathrm{d}z = 1 \tag{4.13}$$

for any fixed vector w with $\|w\| = 1$.

For $x \in [0, 1]$ we define the function $\varphi(x) = -x \ln(x)$ and denote by $\{w_\alpha\}_{\alpha\in\mathbb{N}}$ the eigenbasis of Γ. An application of Jensen's inequality shows

$$\begin{aligned} \operatorname{Tr} \varphi(\Gamma) &= \sum_\alpha \varphi\left(\langle w_\alpha, \Gamma w_\alpha \rangle\right) = \sum_\alpha \varphi\left(\int_{\mathbb{C}} \sum_{\alpha'} g_{\alpha'}(z) |\langle w_\alpha, z \otimes v_{\alpha'}(z) \rangle|^2 p(z) \, \mathrm{d}z \right) \\ &\geq \sum_\alpha \int_{\mathbb{C}} \sum_{\alpha'} \varphi(g_{\alpha'}(z)p(z)) |\langle w_\alpha, z \otimes v_{\alpha'}(z) \rangle|^2 \, \mathrm{d}z = \int_{\mathbb{C}} \sum_{\alpha'} \varphi(g_{\alpha'}(z)p(z)) \, \mathrm{d}z. \end{aligned} \tag{4.14}$$

This is justified because $x \mapsto \varphi(x)$ is concave and (4.13) holds. In the last step we used that $\{w_\alpha\}_{\alpha\in\mathbb{N}}$ is a complete orthonormal basis. With $xy \ln(xy) = xy \ln(x) + xy \ln(y)$ for $x, y \geq 0$ and $\sum_{\alpha'} g_{\alpha'}(z) = 1$, we see that the r.h.s. of (4.14) equals the r.h.s. of the inequality in (4.11), which proves the claim. □

An application of Lemma 4.3 on the r.h.s. of (4.9) and the additivity of the entropy w.r.t. tensor products prove Proposition 4.1.

5. Proof of the main results

Propositions 3.1 and 4.1 imply the following upper bound for the free energy of our trial state:

$$\begin{aligned}\mathrm{Tr}[\mathcal{H}_N\Gamma] - \frac{1}{\beta}S(\Gamma) \leq &\sum_{p\in P_{\mathrm{I}}} p^2\, \mathrm{Tr}_{\mathscr{F}_{\mathrm{I}}}[a_p^* a_p G_{\mathrm{free}}] - \frac{1}{\beta}S(G_{\mathrm{free}}) + \int_{\mathbb{C}} \Big(\mathrm{Tr}_{\mathscr{F}_{\mathrm{B}}}[\mathcal{H}^{\mathrm{B}} G_{\mathrm{B}}(z)] - \frac{1}{\beta} S(G_{\mathrm{B}}(z)) \Big) \zeta(z)\, \mathrm{d}z \\ &+ \mu_0 \sum_{p\in P_{\mathrm{B}}} \gamma(p) + \frac{4\pi\mathfrak{a}}{N|\Lambda|}\int_{\mathbb{C}} |z|^4 \zeta(z)\,\mathrm{d}z - \frac{1}{\beta}S(\zeta) \\ &+ \frac{4\pi\mathfrak{a}}{N|\Lambda|}\Big[2\widetilde{N}_0 \sum_{u\in P_{\mathrm{L}}\setminus\{0\}} \gamma(u) + 2\widetilde{N}_0 \sum_{u\in P_{\mathrm{I}}}\gamma(u) + 2\sum_{u,v\in P_{\mathrm{L}}\setminus\{0\}} \gamma(v)\gamma(u) \Big] + L^{-2}\mathcal{E}_{\mathcal{H}_N}. \end{aligned} \tag{5.1}$$

The Bogoliubov Hamiltonian $\mathcal{H}^{\mathrm{B}}$ and the error term $\mathcal{E}_{\mathcal{H}_N}$ are defined in (2.4) and (3.3), respectively. The first two terms on the r.h.s. can be written as

$$\frac{1}{\beta}\sum_{p\in P_{\mathrm{I}}} \ln\Big(1-\exp(-\beta(p^2-\mu_0))\Big) + \mu_0 \sum_{p\in P_{\mathrm{I}}} \frac{1}{\exp(\beta(p^2-\mu_0))-1} \tag{5.2}$$

with μ_0 in (1.11), and an application of Lemma 2.1 shows that the third term equals

$$E_0 + \frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}} \ln\left(1-\exp(-\beta\varepsilon(p))\right). \tag{5.3}$$

We refer to the same lemma also for the definitions of E_0 and $\varepsilon(p)$. One easily checks that E_0 is negative and can be dropped for an upper bound. Let us define

$$\tilde{\varepsilon}(p) = \sqrt{p^2-\mu_0}\sqrt{p^2-\mu_0+16\pi\mathfrak{a}_N\varrho_0}. \tag{5.4}$$

The function $x\mapsto \ln(1-\exp(-x))$ is monotone increasing ($x\geq 0$). This and (3.18) allow us to replace $\hat{v}_N * \hat{f}_N(p)$ in the definition of $\varepsilon(p)$ by $8\pi\mathfrak{a}_N(1+C/N)$. Moreover, a first order Taylor expansion then shows

$$\frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}}\ln\left(1-\exp(-\beta\varepsilon(p))\right) \leq \frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}}\ln\left(1-\exp(-\beta\tilde{\varepsilon}(p))\right) + \frac{CN_0}{L^2N^2}\sum_{p\in P_{\mathrm{B}}} \frac{p^2-\mu_0}{\exp(\beta(p^2-\mu_0))-1}\frac{1}{p^2}. \tag{5.5}$$

Using $(\exp(x)-1)^{-1}\leq 1/x$ for $x\geq 0$ and $\delta_{\mathrm{B}} < 1/3$, we check that the second term on the r.h.s. is bounded by a constant times $1/L^2$. Moreover, from Lemma B.1 we know that

$$\begin{aligned}\frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}}\ln\left(1-\exp(-\beta\tilde{\varepsilon}(p))\right) \leq &\frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}}\ln\Big(1-\exp(-\beta(p^2-\mu_0))\Big) + 8\pi\mathfrak{a}_N\varrho_0\sum_{p\in P_{\mathrm{B}}}\frac{1}{\exp(\beta(p^2-\mu_0))-1} \\ &- \frac{1}{2\beta}\sum_{p\in\Lambda_+^*}\left[\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2}\right)\right] + \frac{C}{L^2}\left(N^{\delta_{\mathrm{B}}}+N^{2/3-\delta_{\mathrm{B}}}\right) \end{aligned} \tag{5.6}$$

holds.

Next, we have a closer look at the first term in the second line of (5.1). In (2.35)–(2.38) we showed

$$\left|\sum_{p\in P_{\mathrm{B}}}\left(\gamma(p) - \frac{1}{\exp(\beta(p^2-\mu_0))-1}\right)\right| \lesssim \frac{N_0L^2}{N\beta} + \frac{N_0^2}{N^2}, \tag{5.7}$$

and hence

$$\mu_0\sum_{p\in P_{\mathrm{B}}}\gamma(p) \leq \mu_0\sum_{p\in P_{\mathrm{B}}}\frac{1}{\exp(\beta(p^2-\mu_0))-1} + CL^{-2}N^{1/3}. \tag{5.8}$$

To obtain the second bound we also used $-\mu_0 = \ln(1+1/N_0)/\beta \leq 1/(\beta N_0)$ (which follows from (1.12)). In combination, the considerations in (5.2)–(5.8) and $\delta_B < 1/3$ imply

$$
\begin{aligned}
&\sum_{p \in P_{\mathrm{I}}} p^2 \operatorname{Tr}_{\mathscr{F}_{\mathrm{I}}}[a_p^* a_p G_{\mathrm{free}}] - \frac{1}{\beta} S(G_{\mathrm{free}}) + \int_{\mathbb{C}} \left(\operatorname{Tr}_{\mathscr{F}_{\mathrm{B}}}[\mathcal{H}^{\mathrm{B}} G_{\mathrm{B}}(z)] - \frac{1}{\beta} S(G_{\mathrm{B}}(z)) \right) \zeta(z)\, \mathrm{d}z + \mu_0 \sum_{p \in P_{\mathrm{B}}} \gamma(p) \\
&\leq \frac{1}{\beta} \sum_{p \in P_{\mathrm{L}} \backslash \{0\}} \ln\left(1 - \exp(-\beta(p^2 - \mu_0))\right) + \sum_{p \in P_{\mathrm{L}} \backslash \{0\}} \frac{\mu_0}{\exp(\beta(p^2 - \mu_0)) - 1} + \sum_{p \in P_{\mathrm{B}}} \frac{8\pi \mathfrak{a}_N \varrho_0}{\exp(\beta(p^2 - \mu_0)) - 1} \\
&\quad - \frac{1}{2\beta} \sum_{p \in \Lambda_+^*} \left[\frac{16\pi \mathfrak{a}_N \varrho_0(\beta, N, L)}{p^2} - \ln\left(1 + \frac{16\pi \mathfrak{a}_N \varrho_0(\beta, N, L)}{p^2}\right)\right] + CL^{-2}(N^{1/3} + N^{2/3-\delta_{\mathrm{B}}}). \qquad (5.9)
\end{aligned}
$$

In the first two terms on the r.h.s. it remains to replace the sums over $P_{\mathrm{L}} \backslash \{0\}$ by sums over Λ_+^*. One easily checks that this can be done at the expense of an error term that is bounded by a constant times $L^{-2} \exp(-cN^{2\delta_{\mathrm{L}}})$ with some $c > 0$.

The second and the third term in the second line of (5.1) equal

$$
F^{\mathrm{BEC}}(\beta, \widetilde{N}_0, L, \mathfrak{a}_N) = -\frac{1}{\beta} \ln\left(\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi \mathfrak{a}_N L^{-3} |z|^4 - \widetilde{\mu}|z|^2\right)\right) \mathrm{d}z \right) + \widetilde{\mu} \widetilde{N}_0, \qquad (5.10)
$$

where the chemical potential $\widetilde{\mu}$ is chosen such that the Gibbs distribution ζ in (2.7) satisfies (2.9). The first term on the r.h.s. is a concave function of $\widetilde{\mu}$. But this implies

$$
\begin{aligned}
-\frac{1}{\beta} \ln\left(\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi \mathfrak{a}_N L^{-3} |z|^4 - \widetilde{\mu}|z|^2\right)\right) \mathrm{d}z \right) \leq -\frac{1}{\beta} \ln\left(\int_{\mathbb{C}} \exp\left(-\beta\left(4\pi \mathfrak{a}_N L^{-3} |z|^4 - \mu|z|^2\right)\right) \mathrm{d}z \right) + \mu N_0 \\
- \widetilde{\mu} N_0. \qquad (5.11)
\end{aligned}
$$

Here we also used that the first derivative of the first term on the r.h.s. equals $-N_0$.

The identity $\widetilde{N}_0 + \sum_{p \in P_{\mathrm{L}} \backslash \{0\}} \gamma(p) = N$ allows us to write the terms in the third line of (5.1) plus the third term on the r.h.s. of (5.9) as

$$
\frac{4\pi \mathfrak{a}}{N|\Lambda|}\left[2N^2 - 2N_0^2 + 2(N_0^2 - \widetilde{N}_0^2) + 2N_0 \sum_{p \in P_{\mathrm{B}}} \frac{1}{\exp(\beta(p^2 - \mu_0)) - 1} - 2\widetilde{N}_0 \sum_{u \in P_{\mathrm{B}}} \gamma(u)\right]. \qquad (5.12)
$$

In the following, we denote $\gamma_0(p) = \exp(\beta(p^2 - \mu_0) - 1)^{-1}$. Another algebraic manipulation, equations (2.28), (2.21) and (5.7), the bound $\sum_{p \in P_{\mathrm{L}}^c} \gamma(p) \lesssim \exp(-cN^{2\delta_{\mathrm{L}}})$ for some $c > 0$, and $\delta_{\mathrm{L}} > 0$ imply

$$
\begin{aligned}
N_0^2 - \widetilde{N}_0^2 &\leq 2\widetilde{N}_0 \sum_{p \in P_{\mathrm{B}}} (\gamma(p) - \gamma_0(p)) + 2\Big(\sum_{p \in P_{\mathrm{B}}} \gamma(p)\Big) \sum_{p \in P_{\mathrm{B}}} (\gamma(p) - \gamma_0(p)) \\
&\quad + \sum_{p \in P_{\mathrm{B}}} (\gamma_0(p) - \gamma(p)) \sum_{p \in P_{\mathrm{B}}} (\gamma(p) + \gamma_0(p)) + C \exp(-cN^{2\delta_{\mathrm{L}}}) \\
&\leq 2\widetilde{N}_0 \sum_{p \in P_{\mathrm{B}}} (\gamma(p) - \gamma_0(p)) + CN^{4/3+\delta_{\mathrm{B}}}. \qquad (5.13)
\end{aligned}
$$

A similar argument that additionally uses Lemma 2.6 shows

$$
2N_0 \sum_{p \in \mathrm{B}} \gamma_0(p) - 2\widetilde{N}_0 \sum_{p \in P_{\mathrm{B}}} \gamma(p) \leq -2\widetilde{N}_0 \sum_{p \in P_{\mathrm{B}}} (\gamma(p) - \gamma_0(p)) + CN^{4/3+\delta_{\mathrm{B}}}. \qquad (5.14)
$$

When we collect the results in (5.12)–(5.14), we find that (5.12) is bounded from above by

$$
\frac{4\pi \mathfrak{a}}{N|\Lambda|}\left[2N^2 - 2N_0^2\right] + \frac{8\pi \mathfrak{a}}{N|\Lambda|}\left[\widetilde{N}_0 \sum_{p \in P_{\mathrm{B}}} (\gamma(p) - \gamma_0(p))\right] + CL^{-2}N^{1/3+\delta_{\mathrm{B}}}. \qquad (5.15)
$$

We combine now the second term above with the last terms on the r.h. sides of (5.10) and (5.11), that is, we consider

$$\frac{8\pi\mathfrak{a}}{N|\Lambda|}\Big[\widetilde{N}_0 \sum_{p\in P_{\mathrm{B}}} (\gamma(p)-\gamma_0(p))\Big] + \widetilde{\mu}(\widetilde{N}_0 - N_0). \tag{5.16}$$

We distinguish two cases and assume first that $N_0 < N^{5/6+\delta}$ for some $\delta > 0$. In this case applications of (5.7) and Lemma 2.6 show that the first term in (5.16) is bounded by a constant times $L^{-2}N^{1/2+\delta}$. Inspection of (C.6) (recall that $\widetilde{N}_0 = \int |z|^2\zeta(z)\,\mathrm{d}z$ and note that also $\widetilde{N}_0 < N^{5/6+\delta}$, due to Lemma 2.6) shows $|\widetilde{\mu}| \lesssim 1/(\beta\widetilde{N}_0) + \widetilde{N}_0/(L^2N)$. We use this estimate and again Lemma 2.6 to bound the second term in (5.16) by a constant times $L^{-2}N^{1/3+2\delta}$. If $N_0 \geq N^{5/6+\delta}$ we apply part (a) of Lemma C.1 to bound the second term in (5.16) from above by

$$8\pi\mathfrak{a}_N L^{-3}\widetilde{N}_0(\widetilde{N}_0 - N_0) + C\exp(-cN^{\delta}) \leq -8\pi\mathfrak{a}_N L^{-3}\widetilde{N}_0 \sum_{p\in P_{\mathrm{B}}} (\gamma(p)-\gamma_0(p)) + C\exp(-cN^{\delta}) + C\exp(-cN^{2\delta_{\mathrm{L}}}). \tag{5.17}$$

To obtain the second bound, we also used $\sum_{p\in P_{\mathrm{L}}^c} \gamma(p) \lesssim \exp(-cN^{2\delta_{\mathrm{L}}})$ for some $c > 0$. We highlight that the first term on the r.h.s. of (5.17) cancels the first term in (5.16). We collect the above considerations, make the choice $\delta = \delta_{\mathrm{B}}/2 > 0$, and find

$$\frac{8\pi\mathfrak{a}}{N|\Lambda|}\Big[\widetilde{N}_0 \sum_{p\in P_{\mathrm{B}}} (\gamma(p)-\gamma_0(p))\Big] + \widetilde{\mu}(\widetilde{N}_0 - N_0) \lesssim L^{-2}N^{1/3+\delta_{\mathrm{B}}}. \tag{5.18}$$

It remains to collect our results.

In combination, (5.9)–(5.11), (5.15) and (5.18) imply the final upper bound

$$\begin{aligned}\operatorname{Tr}[\mathcal{H}_N\Gamma] - \frac{1}{\beta}S(\Gamma) \leq & \frac{1}{\beta}\sum_{p\in\Lambda_+} \ln\Big(1-\exp(-\beta(p^2-\mu_0))\Big) + \mu_0(N-N_0) + 8\pi\mathfrak{a}_N L^3(\varrho^2-\varrho_0^2) + F^{\mathrm{BEC}}(\beta,N_0,L,\mathfrak{a}_N) \\ & - \frac{1}{2\beta}\sum_{p\in\Lambda_+^*}\left[\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0(\beta,N,L)}{p^2}\right)\right] \\ & + CL^{-2}(N^{1-\delta_{\mathrm{H}}} + N^{\delta_{\mathrm{H}}+2\delta_{\mathrm{B}}} + N^{-1/3+\delta_{\mathrm{H}}+2\delta_{\mathrm{L}}} + N^{1/3+\delta_{\mathrm{B}}} + N^{2/3-\delta_{\mathrm{B}}}).\end{aligned} \tag{5.19}$$

The parameter δ_{L} needs to be strictly positive but can otherwise be chosen as small as we wish. The requirement $\delta_{\mathrm{L}} \leq 1/6$ assures that it plays no role in the optimization. The optimal choice $\delta_{\mathrm{H}} = 1/2 - \delta_{\mathrm{B}}$ with error $N^{1/2+\delta_{\mathrm{B}}}$ follows by combining the first and the second term. Moreover, the optimal choice $\delta_{\mathrm{B}} = 1/12$ results if we combine $N^{1/2+\delta_{\mathrm{B}}}$ and the last term in the last line of (5.19). This leads to an overall error term that is bounded by a constant times $L^{-2}N^{7/12} \ll L^{-2}N^{2/3}$.

As explained in Remark 1.4.(g), the bound in (5.19) is appropriate as long as $N_0 \gg 1$. If $N_0 \sim 1$ the condensate free energy above is strictly larger than F_0^{BEC} in (1.14). We therefore prove a second bound that is appropriate in this parameter regime. As undressed trial state we choose the Gibbs state

$$G_0 = \frac{\exp(-\beta(\,\mathrm{d}\Gamma(-\Delta-\mu_0)))}{\operatorname{Tr}_{\mathscr{F}}[\exp(-\beta(\,\mathrm{d}\Gamma(-\Delta-\mu_0)))]}. \tag{5.20}$$

We define the dressed trial state $\widetilde{\Gamma}$ as in (2.13) with Γ_0 replaced by G_0. To obtain an upper bound for the free energy of $\widetilde{\Gamma}$ we can use a simpler version of the above proof. This is related to the following facts: (a) A coherent state in the definition of our trial state in not needed and the pairing function of G_0 equals zero. (b) The eigenfunctions of G_0 are also eigenfunctions of $\mathrm{d}\Gamma(-\Delta)$. Accordingly, the special treatment of momentum modes in P_{B} at several places in the proof is not needed. We therefore simple state the result and leave further details to the reader:

$$\operatorname{Tr}[\mathcal{H}_N\widetilde{\Gamma}] - \frac{1}{\beta}S(\widetilde{\Gamma}) \leq F_0(\beta,N,L) + 8\pi\mathfrak{a}_N L^3\varrho^2 + CL^{-2}N^{1/2} \tag{5.21}$$

with F_0 defined above (1.14).

We are now prepared to provide the missing proofs in Section 1.6. Theorem 1.1 follows from (5.19), (5.21) and fact that the absolute value of the term in the second line of (5.19) is bounded by a constant times $N_0^2/(\beta N^2)$. The proof of Proposition 1.2 is provided in Appendix C, see Proposition C.2. Finally, Corollary 1.3 is a direct consequence of (5.19), (5.21) and Proposition 1.2.

Acknowledgments. A. D. gratefully acknowledges funding from the Swiss National Science Foundation (SNSF) through the Ambizione grant PZ00P2 185851. It is our pleasure to thank Marco Caporaletti, Phan Thành Nam, Marcin Napiórkowski and Robert Seiringer for inspiring discussions.

— Appendix —

A. The scattering equation

In this appendix we collect some known properties of the finite volume scattering equation (2.10). It is convenient to define $f(Nx) = f_N(x)$, where f satisfies the eigenvalue equation

$$\Big[-\Delta + \frac{v}{2}\Big] f = \lambda_\ell f \tag{A.1}$$

on the ball $|x| \leq N\ell$ with Neumann boundary conditions. It is normalized such that $f(x) = 1$ holds for $|x| = N\ell$. By scaling, we have $N^2\lambda_\ell = \lambda_N$. In the next Lemma we collect the properties of f_N, f and λ_ℓ that are useful for our analysis. The proof can be found in [12, Appendix A].

Lemma A.1. *Let $v \in L^3(\mathbb{R}^3)$ be nonnegative, compactly supported and spherically symmetric. Fix $0 < \ell < L/2$ and let f denote the solution to (A.1) and f_N the solution to (2.10). For $N \in \mathbb{N}$ large enough the following properties hold true.*

1. *We have*
$$\lambda_\ell = \frac{3\mathfrak{a}}{(N\ell)^3}(1 + O(\mathfrak{a}/\ell N)). \tag{A.2}$$

2. *We have $0 \leq f_\ell \leq 1$. Moreover there exists a constant $C > 0$ such that*
$$\Big| \int v(x) f(x) dx - 8\pi\mathfrak{a} \Big| \leq \frac{C\mathfrak{a}^2}{N\ell}. \tag{A.3}$$

3. *There exists a constant $C > 0$ such that, for all $x \in \mathbb{R}^3$,*
$$1 - f(x) \leq \frac{C}{1 + |x|} \quad \textit{and} \quad |\nabla f(x)| \leq \frac{C}{1 + x^2}. \tag{A.4}$$

4. *There exists a constant $C > 0$ such that, for all $p \in \Lambda_+^*$,*
$$\big| \widehat{(1 - f_N)}(p) \big| \leq \frac{C}{Np^2}. \tag{A.5}$$

By definition (2.11), the function $\eta_p = -\widehat{(1 - f_N)}(p)$ solves the equation

$$p^2\eta_p + \frac{\hat{v}_N(p)}{2} + \frac{1}{2|\Lambda|} \sum_{q \in \Lambda^*} \hat{v}_N(p - q)\eta_q = \frac{\lambda_N}{|\Lambda|} \sum_{q \in \Lambda^*} \hat{f}_N(p - q)\hat{\mathbb{1}}_{|x| \leq \ell}(q), \tag{A.6}$$

where $\hat{\mathbb{1}}_{|x|\leq\ell}(q)$ is the Fourier coefficient of the characteristic function of the ball with radius ℓ. Note that we have reinstated units in (A.6). Moreover, by (A.4) and (A.5) we have

$$|\eta_p| \lesssim \frac{L}{Np^2}. \tag{A.7}$$

Inequality (A.7) implies

$$\sum_{p\in\Lambda_+^*:|p|\geq\frac{1}{2L}N^{1-\delta_{\mathrm{H}}}} |\eta_p|^2 \lesssim L^6 N^{-3+\delta_{\mathrm{H}}} \tag{A.8}$$

as well as

$$\sum_{p\in P_{\mathrm{H}}^{\mathrm{c}}} |\eta_p| \lesssim L^3 N^{-\delta_{\mathrm{H}}}, \tag{A.9}$$

where $P_{\mathrm{H}}^{\mathrm{c}}$ denotes the complement of P_{H} in (2.1).

B. Bogoliubov free energy

The goal of this section is to prove the following lemma.

Lemma B.1. *We consider the limit $N\to\infty$, $\beta=\kappa\beta_{\mathrm{c}}$ with $\kappa\in(0,\infty)$ and β_{c} in (1.13). Recall definition (5.4) for $\tilde{\varepsilon}(p)$. There exists a constant $C>0$ such that*

$$\begin{aligned}\frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}} \ln\left(1-\exp(-\beta\tilde{\varepsilon}(p))\right) \leq & \frac{1}{\beta}\sum_{p\in P_{\mathrm{B}}} \ln\Big(1-\exp(-\beta(p^2-\mu_0))\Big) + 8\pi\mathfrak{a}_N\varrho_0 \sum_{p\in P_{\mathrm{B}}} \frac{1}{\exp(\beta(p^2-\mu_0))-1} \\ & - \frac{1}{2\beta}\sum_{p\in\Lambda_+^*}\left[\frac{16\pi\mathfrak{a}_N\varrho_0}{p^2} - \ln\left(1+\frac{16\pi\mathfrak{a}_N\varrho_0}{p^2}\right)\right] + \frac{CN_0^2}{N^2}\left[\frac{N^{\delta_{\mathrm{B}}}}{L^2}+\frac{1}{\beta N^{\delta_{\mathrm{B}}}}+\frac{L^2}{\beta^2 N_0}\right].\end{aligned} \tag{B.1}$$

Proof. We first assume $\mu_0=0$ and then comment on how to adjust the proof to $\mu_0<0$. Let us define the function

$$F(\alpha) = \sum_{p\in\beta^{1/2}P_{\mathrm{B}}} \ln\left(1-\exp\left(-|p|\sqrt{p^2+\alpha}\right)\right). \tag{B.2}$$

For $\alpha=16\pi\mathfrak{a}_N\varrho_0\beta$ it equals β times the l.h.s. of (B.1). In the following we derive an asymptotic expansion of F for small values of α. We also define the functions

$$g_1(x) = \frac{1}{\exp(x)-1} \quad \text{and} \quad g_2(x) = -\frac{1}{4\sinh^2(x/2)} \tag{B.3}$$

and note that the bounds

$$g_1(x) \geq \frac{1}{x} - C \quad \text{and} \quad g_2(x) \leq \frac{-1}{x^2} + \frac{C}{x} \tag{B.4}$$

hold for $0<x\leq 1$. The first and the second derivative of F can be written in terms of g_1 and g_2 as

$$\begin{aligned} F'(\alpha) &= \sum_{p\in\beta^{1/2}P_{\mathrm{B}}} g_1\left(|p|\sqrt{p^2+\alpha}\right)\frac{|p|}{2\sqrt{p^2+\alpha}}, \\ F''(\alpha) &= \frac{1}{4}\sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\left[g_2\left(|p|\sqrt{p^2+\alpha}\right)\frac{p^2}{p^2+\alpha} - g_1\left(|p|\sqrt{p^2+\alpha}\right)\frac{|p|}{(p^2+\alpha)^{3/2}}\right], \end{aligned} \tag{B.5}$$

and hence

$$F(\alpha)-F(0)-F'(0)\alpha=\frac{1}{4}\int_0^\alpha \sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\left[g_2\left(|p|\sqrt{p^2+t}\right)\frac{p^2}{p^2+t}-g_1\left(|p|\sqrt{p^2+t}\right)\frac{|p|}{(p^2+t)^{3/2}}\right](\alpha-t)\,\mathrm{d}t. \tag{B.6}$$

It remains to investigate the r.h.s. of this above identity.

Using the bounds in (B.4), we see that it is bounded from above by

$$-\frac{1}{2}\int_0^\alpha \sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\frac{(\alpha-t)}{(p^2+t)^2}\,\mathrm{d}t+C\alpha\int_0^\alpha \sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\frac{|p|}{(p^2+t)^{3/2}}\,\mathrm{d}t. \tag{B.7}$$

Here, the integral in the second term is bounded by

$$\sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\int_0^\alpha \frac{1}{p^2+t}\,\mathrm{d}t=\sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\ln\left(1+\frac{\alpha}{p^2}\right)\leq \sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\frac{\alpha}{p^2}\lesssim\frac{L^2\alpha N^{\delta_{\mathrm{B}}}}{\beta}. \tag{B.8}$$

A straightforward computation also shows

$$\int_0^\alpha \frac{(\alpha-t)}{(p^2+t)^2}\,\mathrm{d}t=\frac{\alpha}{p^2}-\ln\left(1+\frac{\alpha}{p^2}\right). \tag{B.9}$$

In combination, (B.6)–(B.9) imply

$$F(\alpha)-F(0)-F'(0)\alpha\leq-\frac{1}{2}\sum_{p\in\beta^{1/2}P_{\mathrm{B}}}\left[\frac{\alpha}{p^2}-\ln\left(1+\frac{\alpha}{p^2}\right)\right]+\frac{CL^2\alpha^2N^{\delta_{\mathrm{B}}}}{\beta}. \tag{B.10}$$

Finally, using $\ln(1+x)\geq x-x^2/2$ for $x\geq 0$ we see that

$$\sum_{p\in\beta^{1/2}P_{\mathrm{B}}^{\mathrm{c}}}\left[\frac{\alpha}{p^2}-\ln\left(1+\frac{\alpha}{p^2}\right)\right]\leq\frac{\alpha^2}{2\beta^2}\sum_{p\in P_{\mathrm{B}}^{\mathrm{c}}}\frac{1}{p^4}\lesssim\frac{\alpha^2L^4}{\beta^2N^{\delta_{\mathrm{B}}}}. \tag{B.11}$$

When we put our findings together, we obtain a proof of (B.1) if $\mu_0=0$ (the last error term excluded).

If $\mu_0<0$ our proof applies without changes and we obtain the first term in the second line of (B.1) with p^2 replaced by $p^2-\mu_0$. It is not difficult to check that the difference between these two terms is bounded by a constant times $N_0L^2/(\beta^2N^2)$, which proves the claim of the lemma. □

C. Properties of the free energy of the condensate

In this appendix we prove several statements concerning the effective condensate free energy in (1.17), one of which is Proposition 1.2. The other statements are needed for the proof of Theorem 1.1. We start our discussion with a lemma that provides us with the asymptotic behavior of the chemical potential.

Lemma C.1. *We consider the limit $N\to\infty$, $\beta=\kappa\beta_{\mathrm{c}}$ with $\kappa\in(0,\infty)$ and β_{c} in (1.13). Let g be the Gibbs distribution in (1.18) and assume that $\int_{\mathbb{C}}|z|^2g(z)\,\mathrm{d}z=M$. The chemical potential μ related to g satisfies the following statements for a given $\varepsilon>0$:*

(a) If $M\gtrsim N^{5/6+\varepsilon}$ then there exists a constant $c>0$ such that

$$\left|\mu-8\pi\mathfrak{a}_NM/L^3\right|\lesssim L^{-2}\exp\left(-cN^{\varepsilon}\right). \tag{C.1}$$

(b) If $M \lesssim N^{5/6-\varepsilon}$ then we have

$$\left|\mu + \frac{1}{\beta M}\right| \lesssim \frac{N^{-2\varepsilon}}{\beta M}. \tag{C.2}$$

Proof. We write the two-dimensional integration over $\mathbb{C}$ w.r.t. the measure $\mathrm{d}z = \mathrm{d}x\,\mathrm{d}y/\pi$ in polar coordinates (r,φ) and afterwards introduce the variable $x = r^2$. This allows us to write

$$M = \int_{\mathbb{C}} |z|^2 g(z)\,\mathrm{d}z = \frac{\int_0^\infty x \exp\left(-\beta\left(hx^2 - \mu x\right)\right)\,\mathrm{d}x}{\int_0^\infty \exp\left(-\beta\left(hx^2 - \mu x\right)\right)\,\mathrm{d}x}, \tag{C.3}$$

where $h = 4\pi\mathfrak{a}_N/L^3 \sim L^{-2}N^{-1}$. A short computation shows the integral in the numerator equals

$$\frac{1}{2\beta h} + \frac{\mu}{4h}\sqrt{\frac{\pi}{\beta h}}\exp\left(\frac{\beta\mu^2}{4h}\right)\operatorname{erfc}\left(-\sqrt{\frac{\beta}{h}}\frac{\mu}{2}\right), \tag{C.4}$$

where $\operatorname{erfc}(x) = (2/\sqrt{\pi})\int_x^\infty \exp(-t^2)\,\mathrm{d}t$ denotes the complementary error function. For the integral in the denominator we find

$$\frac{1}{2}\sqrt{\frac{\pi}{\beta h}}\exp\left(\frac{\beta\mu^2}{4h}\right)\operatorname{erfc}\left(-\sqrt{\frac{\beta}{h}}\frac{\mu}{2}\right). \tag{C.5}$$

Let us introduce the notation $\eta = \mu\sqrt{\beta/(4h)}$. Using (C.4) and (C.5), we bring (C.3) to the form

$$\sqrt{\pi\beta h}M = \frac{1 + \sqrt{\pi}\eta\exp(\eta^2)\operatorname{erfc}(-\eta)}{\exp(\eta^2)\operatorname{erfc}(-\eta)} =: \Upsilon(\eta). \tag{C.6}$$

The function Υ is strictly positive, strictly monotone increasing, and satisfies $\lim_{x\to-\infty}\Upsilon(x) = 0$ as well as $\lim_{x\to\infty}\Upsilon(x) = +\infty$. In the following we study the asymptotic behavior of the (unique) solution to this equation. We start with the parameter regime $M \gtrsim N^{5/6+\varepsilon}$, which implies $\sqrt{\pi\beta h}M \gtrsim N^{\varepsilon}$.

In this case the l.h.s. of (C.6) diverges in the limit $N \to \infty$, and hence $\eta \to \infty$. From [1, Eq. 7.1.13] we know that

$$\frac{1}{x + \sqrt{x^2+2}} < \exp\left(x^2\right)\int_x^\infty \exp\left(-t^2\right)\,\mathrm{d}t \leq \frac{1}{x + \sqrt{x^2 + 4/\pi}} \tag{C.7}$$

holds for $x \geq 0$. In combination with $\operatorname{erfc}(-\eta) = 2 - \operatorname{erfc}(\eta)$, this implies

$$2\exp\left(\eta^2\right) - \frac{2}{\sqrt{\pi}\left(\eta + \sqrt{\eta^2 + 4/\pi}\right)} \leq \exp\left(\eta^2\right)\operatorname{erfc}(-\eta) < 2\exp\left(\eta^2\right) - \frac{2}{\sqrt{\pi}\left(\eta + \sqrt{\eta^2+2}\right)} \tag{C.8}$$

as well as

$$\sqrt{\pi\beta h}M = \frac{1 + \sqrt{\pi}\eta\left[2\exp\left(\eta^2\right) + O(1/\eta)\right]}{2\exp\left(\eta^2\right) + O(1/\eta)}. \tag{C.9}$$

We already know that $\eta \gg 1$, and hence $\eta \simeq \sqrt{\beta h}M$. Using this and our assumption $M \gtrsim N^{5/6+\varepsilon}$, which implies $\eta \gtrsim N^{\varepsilon}$, we easily check that (C.1) holds. It remains to prove (C.2).

If $M \lesssim N^{5/6-\varepsilon}$ the l.h.s. of (C.6) satisfies $\sqrt{\pi\beta h}M \lesssim N^{-\varepsilon}$ and we therefore have $\eta \to -\infty$. To obtain the leading order behavior of η, the approximation provided by (C.7) is not sufficiently accurate. A more precise approximation is provided by [1, Eq. 7.1.23], which implies

$$\sqrt{\pi}\exp(x^2)\operatorname{erfc}(x) = \frac{1}{x} - \frac{1}{2x^3} + Q(x), \quad \text{where } Q \text{ satisfies} \quad |Q(x)| \leq \frac{3}{4x^5} \tag{C.10}$$

for $x \geq 0$. We use this approximation in (C.6) and find

$$\sqrt{\beta h} M = \frac{1}{2|\eta|}\left(1 + O\left(\eta^{-2}\right)\right). \tag{C.11}$$

Eq. (C.2) is a direct consequence of (C.11). This proves our claim. □

We are now prepared to give the proof of Proposition 1.2. Because of technical reasons, we prove it in a slightly more general situation.

Proposition C.2. *We consider the limit $N \to \infty$, $\beta = \kappa\beta_c$ with $\kappa \in (0, \infty)$ and β_c in (1.13). The following statements hold for given $\varepsilon > 0$:*

(a) Assume that $M \gtrsim N^{5/6+\varepsilon}$. There exists a constant $c > 0$ such that

$$F^{\mathrm{BEC}}(\beta, M, L, \mathfrak{a}_N) = 4\pi\mathfrak{a}_N L^{-3} M^2 + \frac{\ln\left(4\beta\mathfrak{a}_N/L^3\right)}{2\beta} + O\left(L^{-2}\exp\left(-cN^{\varepsilon}\right)\right). \tag{C.12}$$

(b) Assume that $M \lesssim N^{5/6-\varepsilon}$. Then

$$F^{\mathrm{BEC}}(\beta, M, L, \mathfrak{a}_N) = -\frac{1}{\beta}\ln(M) - \frac{1}{\beta} + O\left(L^{-2}N^{2/3-2\varepsilon}\right) \tag{C.13}$$

holds. In particular, $F^{\mathrm{BEC}}(\beta, M, L, \mathfrak{a}_N)$ is independent of $\mathfrak{a}_N$ at the given level of accuracy.

Proof. The free energy $F^{\mathrm{BEC}}(\beta, M, L, \mathfrak{a}_N)$ in (1.17) consists of two terms. In the following, we denote the first by $\Phi(\beta, M, L, \mathfrak{a}_N)$. When we apply the same coordinate transformations that led to (C.3), we can write it as

$$\Phi(\beta, M, L, \mathfrak{a}_N) = -\frac{1}{\beta}\ln\left(\int_0^{\infty}\exp\left(-\beta\left(hx^2 - \mu x\right)\right)\mathrm{d}x\right) = -\frac{1}{\beta}\ln\left(\frac{1}{2}\sqrt{\frac{\pi}{\beta h}}\exp\left(\frac{\beta\mu^2}{4h}\right)\mathrm{erfc}\left(-\sqrt{\frac{\beta}{h}}\frac{\mu}{2}\right)\right), \tag{C.14}$$

where the second identity follows from the fact that the denominator in (C.3) is given by (C.5).

We first consider the parameter regime $M \gtrsim N^{5/6+\varepsilon}$, where $\eta \simeq \sqrt{\beta h} M \gtrsim N^{\varepsilon}$. An application of (C.8) shows that the r.h.s. of (C.14) equals

$$-\frac{1}{\beta}\ln\left(\sqrt{\frac{\pi}{\beta h}}\exp(\eta^2)\left(1 + O\left(\exp(-\eta^2)/\eta\right)\right)\right) = \frac{1}{2\beta}\ln\left(\frac{4\beta\mathfrak{a}_N}{L^3}\right) - 4\pi\mathfrak{a}_N M^2 L^{-3} + O\left(L^{-2}\exp\left(-cN^{2\varepsilon}\right)\right). \tag{C.15}$$

From Lemma C.1 we know that

$$\mu M = 8\pi\mathfrak{a}_N M^2 L^{-3} + O\left(L^{-2}\exp\left(-cN^{\varepsilon}\right)\right). \tag{C.16}$$

In combination, these consideration show

$$F^{\mathrm{BEC}}(\beta, M, L, \mathfrak{a}_N) = \Phi(\beta, M, L, \mathfrak{a}_N) + \mu M = \frac{1}{2\beta}\ln\left(\frac{4\beta\mathfrak{a}_N}{L^3}\right) + 4\pi\mathfrak{a}_N M^2 L^{-3} + O\left(L^{-2}\exp\left(-cN^{\varepsilon}\right)\right), \tag{C.17}$$

which proves (C.12).

Next, we consider the case $M \lesssim N^{5/6-\varepsilon}$, where $\eta \simeq -1/(2\sqrt{\beta h}M) \lesssim -N^{\varepsilon}$. We use (C.10) to write Φ as

$$\Phi(\beta, M, L, \mathfrak{a}_N) = -\frac{1}{\beta}\ln\left(\sqrt{\frac{1}{\beta h}}\frac{1}{2|\eta|}\left(1 + O\left(\eta^{-2}\right)\right)\right) = -\frac{\ln(M)}{\beta} + O\left(N^{-2\varepsilon}/\beta\right). \tag{C.18}$$

To obtain the second equality we applied Lemma C.1. Another application of the same lemma yields

$$\mu M = -\frac{1}{\beta}\left(1 + O\left(N^{-2\varepsilon}\right)\right). \tag{C.19}$$

In combination, (C.18) and (C.19) prove (C.13). □

The last lemma provides us with a bound for the moments of the distribution ζ, which is needed in our proof of Lemma 2.8 in Section 2.2. We recall that ζ equals g in (1.18) except that the chemical potential $\widetilde{\mu}$ is chosen s.t. $\int_{\mathbb{C}} |z|^2 \zeta(z)\,\mathrm{d}z = \widetilde{N}_0$ holds with $\widetilde{N}_0$ in (2.9).

Lemma C.3. *We consider the limit $N \to \infty$, $\beta = \kappa\beta_c$ with $\kappa \in (0,\infty)$ and β_c in (1.13). The probability distribution ζ defined below (2.7) satisfies the bound*

$$\int_{\mathbb{C}} |z|^{2k} \zeta(z)\,\mathrm{d}z \lesssim N^k \tag{C.20}$$

for $k \in \{1,2,3,4\}$.

Proof. Let us again use the notation $h = 4\pi\mathfrak{a}_N L^{-3}$. We claim that

$$\int_{\mathbb{C}} |z|^{2n+2} \zeta(z)\,\mathrm{d}z = \frac{\widetilde{\mu}}{2h} \int_{\mathbb{C}} |z|^{2n} \zeta(z)\,\mathrm{d}z + \frac{n}{2\beta h} \int_{\mathbb{C}} |z|^{2n-2} \zeta(z)\,\mathrm{d}z \tag{C.21}$$

holds for $n \geq 1$. To prove this, we first use the same coordinate transformations as above (C.3) and find

$$\int_{\mathbb{C}} |z|^{2k} \zeta(z)\,\mathrm{d}z = \frac{1}{Z} \int_0^\infty x^k \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x \quad \text{with} \quad Z = \int_0^\infty \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x \tag{C.22}$$

for $k \geq 0$. We also have

$$\begin{aligned} \frac{-1}{2\beta h} \int_0^\infty x^n \frac{\mathrm{d}}{\mathrm{d}x} \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x = & \int_0^\infty x^{n+1} \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x \\ & - \frac{\mu}{2h} \int_0^\infty x^n \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x. \end{aligned} \tag{C.23}$$

When we integrate by parts in the first term on the l.h.s. and use $n \geq 1$, this implies

$$\int_0^\infty x^{n+1} \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x = \frac{\widetilde{\mu}}{2h} \int_0^\infty x^n \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x + \frac{n}{2\beta h} \int_0^\infty x^{n-1} \exp(-\beta(hx^2 - \widetilde{\mu}x))\,\mathrm{d}x. \tag{C.24}$$

Eq. (C.21) is a direct consequence of (C.22) and (C.24).

If $\widetilde{\mu} \leq 0$ we have

$$\int_{\mathbb{C}} |z|^{2n+2} \zeta(z)\,\mathrm{d}z \leq \frac{n}{2\beta h} \int_{\mathbb{C}} |z|^{2n-2} \zeta(z)\,\mathrm{d}z \lesssim nN^{5/3} \int_{\mathbb{C}} |z|^{2n-2} \zeta(z)\,\mathrm{d}z, \tag{C.25}$$

where we used $\beta \sim L^2 N^{-2/3}$ to obtain the second inequality. It is easy to check that (C.25), $\int \zeta(z)\,\mathrm{d}z = 1$, and $\int |z|^2 \zeta(z)\,\mathrm{d}z = \widetilde{N}_0 \leq N$ imply (C.20) in this case.

Inspection of (C.6) shows that the chemical potential assumes its largest (positive) values when $\widetilde{N}_0 \sim N$. This follows from the fact that the l.h.s. of (C.6) is strictly increasing in M and that the two maps $\widetilde{\eta} \mapsto \Upsilon(\widetilde{\eta})$ with Υ in (C.6) and $\widetilde{\mu} \mapsto \widetilde{\eta} = \widetilde{\mu}\sqrt{\beta/(4h)}$ are strictly increasing. Application of part (a) of Lemma C.1 and the bound $\widetilde{N}_0 \leq N$ therefore show that $\widetilde{\mu}$ can be bounded by $4\pi\mathfrak{a}_N N L^{-3} \lesssim L^{-2}$. When we use this bound and $\beta \sim L^2 N^{-2/3}$ in (C.21), we find

$$\int_{\mathbb{C}} |z|^{2n+2} \zeta(z)\,\mathrm{d}z \lesssim N \int_{\mathbb{C}} |z|^{2n} \zeta(z)\,\mathrm{d}z + nN^{5/3} \int_{\mathbb{C}} |z|^{2n-2} \zeta(z)\,\mathrm{d}z, \tag{C.26}$$

which implies (C.20) in the case $\mu > 0$. □

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