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The Simplified Approach to the Bose Gas Without Translation Invariance

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Abstract

The simplified approach to the Bose gas was introduced by Lieb in 1963 to study the ground state of systems of interacting Bosons. In a series of recent papers, it has been shown that the simplified approach exceeds earlier expectations, and gives asymptotically accurate predictions at both low and high density. In the intermediate density regime, the qualitative predictions of the simplified approach have also been found to agree very well with quantum Monte Carlo computations. Until now, the simplified approach had only been formulated for translation invariant systems, thus excluding external potentials, and non-periodic boundary conditions. In this paper, we extend the formulation of the simplified approach to a wide class of systems without translation invariance. This also allows us to study observables in translation invariant systems whose computation requires the symmetry to be broken. Such an observable is the momentum distribution, which counts the number of particles in excited states of the Laplacian. In this paper, we show how to compute the momentum distribution in the simplified approach, and show that, for the simple equation, our prediction matches up with Bogolyubov's prediction at low densities, for momenta extending up to the inverse healing length.

Keywords Bose gas · Simplified approach to the Bose gas · Trapped Bosons

1 Introduction

The Bose gas is one of the simplest models in quantum statistical mechanics, and yet it has a rich and complex phenomenology. As such, it has garnered much attention from the mathematical physics community for over half a century. It consists of infinitely many identical Bosons and is used to model a wide range of physical systems, from photons in black body radiation to gasses of helium atoms. Whereas photons do not directly interact with each other, helium atoms do, and such an interaction makes studying such systems very challenging. To account for interactions between Bosons, Bogolyubov [5] introduced a widely used approximation scheme that accurately predicts many observables [23] *in the low density* regime.

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Even though Bogolyubov theory is not mathematically rigorous, it has allowed mathematical physicists to develop the necessary intuition to prove a wide variety of results about the Bose gas, such as the low density expansion of the ground state energy of the Bose gas in the thermodynamic limit [1, 13–16, 34], as well as many other results in scaling limits other than the thermodynamic limit (see [17] for a review, as well as, among many others, [2–4, 6, 7, 11, 12, 19, 27, 28, 30–32]). In this note, we will focus on the ground state in the thermodynamic limit.

In 1963, Lieb [24–26] introduced a new approximation scheme to compute properties of the ground state of Bose gasses, called the *simplified approach*, which has recently been found to yield surprisingly accurate results [8–10, 20]. Indeed, while Bogolyubov theory is accurate at low densities, the simplified approach has been shown to yield asymptotically accurate results at both *low and high* densities [8, 9] for interaction potentials that are of positive type, as well as reproduce the qualitative behavior of the Bose gas at intermediate densities [10]. In addition to providing a promising tool to study the Bose gas, the derivation of the Simplified approach is different enough from Bogolyubov theory that it may give novel insights into longstanding open problems about the Bose gas.

The original derivation of the Simplified approach [24] is quite general, and applies to any translation invariant system (it even works for Coulomb [26] and hard-core [10] interactions). In the present paper, we extend this derivation to systems that break translation invariance. This allows us to formulate the simplified approach for systems with external potentials, and with a large class of boundary conditions. In addition, it allows us to compute observables in systems with translation invariance, but whose computation requires breaking the translation invariance. We will discuss an example of such an observable: the momentum distribution.

The momentum distribution $\mathcal{M}(k)$ is the probability of finding a particle in the state e^{ikx}. Bose gasses are widely expected to form a Bose–Einstein condensate, although this has still not been proven (at least for continuum interacting gasses in the thermodynamic limit). From a mathematical point of view, Bose–Einstein condensation is defined as follows: if the Bose gas consists of N particles, the average number of particles in the constant state (corresponding to $k = 0$ in e^{ikx}) is of order N. The *condensate fraction* is defined as the proportion of particles in the constant state. The momentum distribution is an extension of the condensate fraction to a more general family of states. In particular, computing $\mathcal{M}(k)$ for $k \neq 0$ amounts to counting particles that are *not* in the condensate. This quantity has been used in the recent proof [15, 16] of the energy asymptotics of the Bose gas at low density. A numerical computation of the prediction of the Simplified approach for $\mathcal{M}(k)$ has been published in [22].

The main results in this paper fall into two categories. First, we will derive the simplified approach without assuming translation invariance, see Theorem 1. To do so, we will make the so-called "factorization assumption", on the marginals of the ground state wavefunction, see Assumption 1. This allows us to derive a simplified approach for a wide variety of situations in which translation symmetry breaking is violated, such as in the presence of external potentials. Second, we compute a prediction for the momentum distribution using the simplified approach. The simplified approach does not allow us to compute the ground state wavefunction directly, so to compute observables, such as the momentum distribution, we use the Hellmann–Feynman technique and add an operator to the Hamiltonian. In the case of the momentum distribution, this extra operator is a projector onto e^{ikx}, which breaks the translation invariance of the ground state wavefunctions. In Theorem 2, we show how to compute the momentum distribution in the simplified approach using the general result of Theorem 1. In addition, we check that the prediction is credible, by comparing it to the prediction of Bogolyubov theory, and find that both approaches agree at low densities and small k, see Theorem 3.

The result in this paper concerns the derivation of the Simplified approach for Bose gasses without translation invariance. As of this writing, this derivation has *not* been done in a mathematically rigorous. Doing so is an important open problem (as the predictions of the simplified approach are expansive, even more so than Bogolyubov theory). However, the derivation of the simplified approach in translation invariant settings has also not been derived rigorously, and it would seem that the translation invariant situation will be easier to approach. So justifying the simplified approach in the translation invariant setting may be a more pressing task. That being said, the Simplified approach has proved to have strong predictive power [10, 22], so the extension presented in this paper has the potential to yield interesting physical predictions, as the translation-invariant approach has done (although, in all fairness, the non-translation invariant Simplified approach is computationally more difficult than the translation invariant one). In addition, the derivation of the simplified approach for the trapped Bose gas may shine some light on an extension of Gross–Piatevskii theory beyond low density regimes. Work in this direction is ongoing.

Instead of providing a derivation of the simplified approach from the many-body Bose gas (which is beyond reach at the moment), this paper aims to put the derivation of the simplified approach in non-translation invariant settings on a firm footing, and make clear what is rigorous, and what is an approximation.

The rest of the paper is structured as follows. In Sect. 2, we specify the model and state the main results precisely. We then prove Theorem 1 in Sect. 3, Theorem 2 in Sect. 4.1, and Theorem 3 in Sect. 4.2. The proofs are largely independent and can be read in any order.

2 The Model and Main Results

Consider N Bosons in a box of volume V denoted by $\Omega_V := [-V^{\frac{1}{3}}/2, V^{\frac{1}{3}}/2]^3$, interacting with each other via a pair potential $v \in L_1(\Omega_V^2)$ that is symmetric under exchanges of particles: $v(x,y) \equiv v(y,x)$ and non-negative: $v(x,y) \geqslant 0$. The Hamiltonian acts on $L_{2,\mathrm{sym}}(\Omega_V^N)$ as

$$\mathcal{H} := -\frac{1}{2}\sum_{i=1}^N \Delta_i + \sum_{1\leqslant i<j\leqslant N} v(x_i,x_j) + \sum_{i=1}^N P_i \tag{1}$$

where $\Delta_i \equiv \partial_{x_i}^2$ is the Laplacian with respect to the position of the i-th particle and P_i is an extra single-particle term of the following form: given a self-adjoint operator ϖ on $L_2(\Omega_V)$,

$$P_i := \mathbb{1}^{\otimes i-1} \otimes \varpi \otimes \mathbb{1}^{\otimes N-i}. \tag{2}$$

ϖ can be chosen to be any self-adjoint operator, as long as $\mathcal{H}$ is self-adjoint. For instance, if we take ϖ to be a multiplication operator by a function $v_0 \geqslant 0$, then $\sum_i P_i$ is the contribution of the external potential v_0. In particular, this potential could be taken to scale with the volume of the box V, as in the Gross-Pitaevskii approach [18, 33]. Alternatively, v_0 could be taken to be a periodic external potential. Or ϖ could be a projector onto e^{ikx}, which is what we will do below to compute the momentum distribution. Because P_i acts on a single particle, it can prevent H from being translation invariant (which is the case when ϖ is the multiplication operator by $v_0 > 0$). But even if it does not, because the ground states can be degenerate in the presence of P_i (see below), the translation invariance of the Hamiltonian does not necessarily translate into the translation invariance of the ground states.

We may impose any boundary condition on the box, as long as the Laplacian is self-adjoint. We will consider the thermodynamic limit, in which $N, V \to \infty$, such that

$$\frac{N}{V} = \rho \tag{3}$$

is fixed. We consider a ground state ψ_0, which is an eigenfunction of $\mathcal{H}$ with the lowest eigenvalue E_0:

$$\mathcal{H}\psi_0 = E_0\psi_0. \tag{4}$$

When the operator ϖ is a multiplication operator by a function $v_0 \geqslant 0$ (that is, when it is a single-body potential), the ground state is unique, real, and non-negative (this follows from the Perron–Frobenius theorem and the fact that v and v_0 are non-negative, see e.g. [21, Exercise E5]). In more general settings, this is not necessarily the case. In such a case, the Simplified approach should be approximating the properties of *one* of the ground states, but gives no control over which one it is: as will be apparent below, the derivation of the Simplified approach does not depend on which eigenstate ψ_0 is, just on the factorization Assumption 1.

This is not to say that the Simplified approach applies to *all* eigenstates, or even to all ground states. The crucial assumption in the simplified approach is the factorization assumption 1. As we will discuss in more detail below, this is actually an *approximation* rather than an assumption, since it can be shown that it cannot possibly hold exactly for *any* wavefunction. As such, understanding which states best approximately satisfy the factorization assumption is not an easy task. For this reason, we will remain agnostic so as to which of the ground state is studied.

In order to take the thermodynamic limit, we will assume that v is uniformly integrable in V:

$$|v(x, y)| \leqslant \bar v(x, y), \quad \int_{\mathbb{R}^3} dy\ \bar v(x, y) \leqslant c \tag{5}$$

where $\bar v$ and c are independent of V. In addition, we assume that, for any f that is uniformly integrable in V,

$$\int dx\ \varpi f(x) \leqslant c. \tag{6}$$

2.1 The Simplified Approach Without Translation Invariance

The crucial idea of Lieb's construction [24] is to consider the wave function ψ_0 as a probability distribution, instead of the usual $|\psi_0|^2$. When ϖ is the multiplication by $v_0 \geqslant 0$, $\psi_0 \geqslant 0$, so ψ_0, normalized by its L_1 norm, is indeed a probability distribution. In other cases, the probabilistic interpretation of ψ_0 falls through, and the factorization assumption 1 can no longer be interpreted in terms of statistical independence. We then define the i-th marginal of ψ_0 as

$$\mathfrak{g}_i(x_1, \cdots, x_i) := \frac{\int \frac{dx_{i+1}}{V} \dots \frac{dx_N}{V}\ \psi_0(x_1, \dots, x_N)}{\int \frac{dy_1}{V} \dots \frac{dy_N}{V}\ \psi_0(y_1, \dots, y_N)} \tag{7}$$

that is

$$\mathfrak{g}_i(x_1, \dots, x_i) \equiv V^i \frac{\int dx_{i+1} \cdots dx_N\ \psi_0(x_1, \dots, x_N)}{\int dy_1 \dots dy_N\ \psi_0(y_1, \dots, y_N)}. \tag{8}$$

In particular, for $i \in \{2, \ldots, N\}$,

$$\int \frac{dx_i}{V}\, \mathfrak{g}_i(x_1, \ldots, x_i) = \mathfrak{g}_{i-1}(x_1, \ldots, x_{i-1}), \quad \int \frac{dx}{V}\, \mathfrak{g}_1(x) = 1. \tag{9}$$

Because of the symmetry of ψ_0 under exchanges of particles, $\mathfrak{g}_i$ is symmetric under $x_i \leftrightarrow x_j$.

Remark: If the ground state is not unique, then there may be choices of ψ_0 that are orthogonal to the constant wavefunction, that is, that integrate to 0: $\int dy_1 \ldots dy_N\, \psi_0(y_1, \ldots, y_N) = 0$. The derivation in this paper precludes such a possibility, as $\mathfrak{g}_i$ would be ill defined. We will therefore assume that ψ_0 has non-trivial overlap with the constant wavefunction: $\int dy_1 \ldots dy_N\, \psi_0(y_1, \ldots, y_N) \neq 0$ (which is certainly the case whenever the ground state is non-negative).

We rewrite (4) as a family of equations for $\mathfrak{g}_i$.

1. Integrating (4) with respect to $x_1, \ldots, x_N$, we find that

$$E_0 = G_0^{(2)} + F_0^{(1)} + B_0 \tag{10}$$

with

$$G_0^{(2)} := \frac{N(N-1)}{2V^2} \int dxdy\, v(x,y)\mathfrak{g}_2(x,y) \tag{11}$$

$$F_0^{(1)} := \frac{N}{V} \int dx\, \varpi \mathfrak{g}_1(x) \tag{12}$$

and B_0 is a boundary term:

$$B_0 = -\frac{N}{2V} \int dx\, \Delta \mathfrak{g}_1(x). \tag{13}$$

2. If, now, we integrate (4) with respect to $x_2, \ldots, x_N$, we find

$$-\frac{\Delta}{2}\mathfrak{g}_1(x) + \varpi \mathfrak{g}_1(x) + G_1^{(2)}(x) + G_1^{(3)}(x) + F_1^{(2)}(x) + B_1(x) = E_0 \mathfrak{g}_1(x) \tag{14}$$

with

$$G_1^{(2)}(x) := \frac{N-1}{V} \int dy\, v(x,y)\mathfrak{g}_2(x,y) \tag{15}$$

$$G_1^{(3)}(x) := \frac{(N-1)(N-2)}{2V^2} \int dydz\, v(y,z)\mathfrak{g}_3(x,y,z) \tag{16}$$

$$F_1^{(2)}(x) := \frac{N-1}{V} \int dy\, \varpi_y \mathfrak{g}_2(x,y) \tag{17}$$

in which we use the notation ϖ_y to indicate that ϖ applies to $y \mapsto \mathfrak{g}_2(x,y)$, and B_1 is a boundary term

$$B_1(x) := -\frac{N-1}{2V} \int dy\, \Delta_y \mathfrak{g}_2(x,y). \tag{18}$$

3. If we integrate with respect to $x_3, \ldots, x_N$, we find

$$-\frac{1}{2}(\Delta_x + \Delta_y)\mathfrak{g}_2(x,y) + v(x,y)\mathfrak{g}_2(x,y) + (\varpi_y + \varpi_x)\mathfrak{g}_2(x,y) + \\ + G_2^{(3)}(x,y) + G_2^{(4)}(x,y) + F_2^{(3)}(x,y) + B_2(x,y) = E_0 \mathfrak{g}_2(x,y) \tag{19}$$

where, here again, ϖ_y indicates that ϖ applies to the y-degree of freedom, whereas ϖ_x applies to x, with

$$G_2^{(3)}(x,y) := \frac{N-2}{V}\int dz\ (v(x,z)+v(y,z))\mathfrak{g}_3(x,y,z) \tag{20}$$

$$G_2^{(4)}(x,y) := \frac{(N-2)(N-3)}{2V^2}\int dzdt\ v(z,t)\mathfrak{g}_4(x,y,z,t) \tag{21}$$

$$F_2^{(3)}(x,y) := \frac{N-2}{V}\int dz\ \varpi_z\mathfrak{g}_3(x,y,z) \tag{22}$$

and B_2 is a boundary term

$$B_2(x) := -\frac{N-2}{2V}\int dz\ \Delta_z\mathfrak{g}_3(x,y,z). \tag{23}$$

Inspired by [24], we will make the following approximation.

Assumption 1 (*Factorization*) We will approximate $\mathfrak{g}_i$ by functions g_i, which satisfy the following:

$$g_2(x,y) = g_1(x)g_1(y)(1-u_2(x,y)) \tag{24}$$

and for $i=3,4$,

$$g_i(x_1,\ldots,x_i) = \prod_{1\leqslant j<l\leqslant i} W_i(x_j,x_l) \tag{25}$$

with

$$W_i(x,y) = f_i(x)f_i(y)(1-u_i(x,y)) \tag{26}$$

in which, for $i=2,3,4$ and $j=3,4$, f_j and u_i are bounded independently of V, $f_i\geqslant 0$, and u_i is uniformly integrable in V:

$$|u_i(x,y)| \leqslant \bar u_i(x,y), \quad \int dy\ \bar u_i(x,y) \leqslant c_i \tag{27}$$

with c_i independent of V. We further assume that, for $i=1,2,3$, $\forall x_1,\ldots,x_{i-1}$,

$$\lim_{V\to\infty}\int dx_i\ \Delta_{x_i}g_i(x_1,\ldots,x_i) = 0 \tag{28}$$

in other words, these boundary terms vanish in the thermodynamic limit (these are indeed boundary terms by the divergence theorem).

In other words, g_i factorizes exactly as a product of pair terms W_i. The f_i in W_i allow for W_i to be modulated by a slowly varying density, which is the main novelty of this paper compared to [24]. The inequality (27) ensures that u_i decays sufficiently fast on the microscopic scale. Note that, by the symmetry under exchanges of particles, $u_i(x,y)\equiv u_i(y,x)$.

Note, in addition, that assumption (24) is less general than (25): we impose that, as x and y are far from each other, g_2 converges to $g_1(x)g_1(y)$. This is necessary: if we merely assumed that $g_2(x,y) = f_2(x)f_2(y)(1-u_2(x,y))$, we would not necessarily recover that $f_2 = g_1$. However, as we will show below, assumption 1 does imply that $f_3 = g_1$ and $f_4 = g_1$ (up to corrections in V^{-1} that are irrelevant).

Here, we use the term "assumption" because it leads to the simplified approach. However, it is really an *approximation* rather than an assumption: this factorization will certainly not hold true exactly. At best, one might expect that the assumption holds approximately in the limit of small and large ρ, and for distant points, as numerical evidence suggests in the translation invariant case. In the present paper, we will not attempt a proof that this approximation is accurate, and instead explore its consequences. Suffice it to say that this approximation is one of *statistical independence* that is reminiscent of phenomena arising in statistical mechanics when the density is low, that is, when the interparticle distances are large. In the current state of the art, we do not have much in the way of an explanation for why this statistical independence should hold (especially in cases where ψ_0 is not even non-negative); instead, we have extensive evidence, both numerical [10] and analytical [8, 9], that this approximation leads to very accurate predictions.

From this point on, we will make no further approximations, and derive the consequences of assumption 1 in a mathematically rigorous way. This thus makes clear what is an approximation, and what is not.

The equations of the Simplified approach are derived from Assumption 1, using the eigenvalue Eq. (4) along with

$$\int \frac{dx}{V}\, g_1(x) = 1 \tag{29}$$

$$\int \frac{dy}{V}\, g_2(x, y) = g_1(x) \tag{30}$$

$$\int \frac{dz}{V}\, g_3(x, y, z) = g_2(x, y) \tag{31}$$

$$\int \frac{dz}{V}\frac{dt}{V}\, g_4(x, y, z, t) = g_2(x, y) \tag{32}$$

(all of which hold for $\mathfrak{g}_i$, by (9)) to compute u_i and f_i.

In the translation invariant case, the factorization assumption leads to an equation for g_2 alone, as g_1 is constant. When translation invariance is broken, g_1 is no longer constant, and the simplified approach consists in two coupled equations for g_1 and g_2.

Theorem 1 *If g_i satisfies Assumption 1, the Eqs. (14) and (19) with $\mathfrak{g}_1$ replaced by g_1 and $\mathfrak{g}_2$ by g_2, as well as (29)–(32), then g_1 and u_2 satisfy the two coupled equations*

$$\begin{aligned}&\left(-\frac{\Delta}{2} + (\varpi - \langle\varpi\rangle) + 2\,(\mathcal{E}(x) - \langle\mathcal{E}(y)\rangle) + \frac{1}{2}\left(\bar{A}(x) - \left\langle\bar{A}\right\rangle - \bar{C}(x)\right)\right) g_1(x)\\ &+\Sigma_1(x) = 0\end{aligned} \tag{33}$$

and

$$\begin{aligned}&\left(-\frac{1}{2}(\Delta_x + \Delta_y) + v(x, y) - 2\rho\bar{K}(x, y) + \rho^2\bar{L}(x, y) + \bar{R}_2(x, y)\right)\\ &\cdot g_1(x)g_1(y)(1 - u_2(x, y)) + \Sigma_2(x, y) = 0\end{aligned} \tag{34}$$

where

$$\langle f\rangle := \int \frac{dy}{V}\, g_1(y)f(y), \quad \langle\varpi\rangle \equiv \int \frac{dy}{V}\,\varpi g_1(y) \tag{35}$$

$$\bar S(x,y) := v(x,y)(1-u_2(x,y)), \quad f_1\bar{*}f_2(x,y) := \int dz\ g_1(z)f_1(x,z)f_2(z,y) \tag{36}$$

$$\mathcal{E}(x) := \frac{\rho}{2}\int dy\ g_1(y)\bar S(x,y), \quad \bar A(x) := \rho^2\bar S\bar{*}u_2\bar{*}u_2(x,x) \tag{37}$$

$$\bar C(x) := 2\rho^2\int dz\ g_1(z)u_2\bar{*}\bar S(x,z) + 2\rho\int dy\ \varpi_y(g_1(y)u_2(x,y)). \tag{38}$$

$$\bar K(x,y) := \bar S\bar{*}u_2(x,y) \tag{39}$$

$$\bar L(x,y) := \bar S\bar{*}u_2\bar{*}u_2(x,y) - 2u_2\bar{*}(u_2(u_2\bar{*}\bar S))(x,y) + \frac{1}{2}\int dzdt\ g_1(z)g_1(t)\bar S(z,t)u_2(x,z)u_2(x,t)u_2(y,z)u_2(y,t) \tag{40}$$

$$\begin{aligned}\bar R_2(x,y) = {} & 2\left(\mathcal{E}(x)+\mathcal{E}(y)-2\langle\mathcal{E}\rangle\right) + \left(\varpi_x+\varpi_y-2\langle\varpi\rangle\right)\\ & +\frac{1}{2}\left(\bar A(x)+\bar A(y)-2\langle\bar A\rangle - \bar C(x)-\bar C(y)\right) + 2\rho u_2\bar{*}\left(u_2(\mathcal{E}-\langle\mathcal{E}\rangle)\right)\\ & +\rho\int dz\ \varpi_z(g_1(z)u_2(x,z)u_2(y,z)) - \rho u_2\bar{*}u_2\langle\varpi\rangle\end{aligned} \tag{41}$$

in which ϖ_x is the action of ϖ on the x-variable, and similarly for ϖ_y and

$$\Sigma_i \xrightarrow[V\to\infty]{} 0 \tag{42}$$

pointwise. The prediction for the energy per particle is defined as

$$e := \langle\mathcal{E}\rangle + \langle\varpi\rangle + \Sigma_0 \tag{43}$$

where $\Sigma_0 \to 0$ as $V\to\infty$.

This theorem is proved in Sect. 3.

Let us compare this to the equation for u in the Simplified approach in the translation invariant case [10, (5)], [20, (3.15)]:

$$-\Delta u(x) = (1-u(x))\left(v(x)-2\rho K(x)+\rho^2 L(x)\right) \tag{44}$$

$$K := u*S, \quad S(y) := (1-u(y))v(y) \tag{45}$$

$$L := u*u*S - 2u*(u(u*S)) + \frac{1}{2}\int dydz\ u(y)u(z-x)u(z)u(y-x)S(z-y). \tag{46}$$

We will prove that these follow from Theorem 1:

Corollary 1 (Translation invariant case) *In the translation invariant case $v(x,y)\equiv v(x-y)$ and $\varpi=0$ with periodic boundary conditions, if* (33)–(34) *has a unique translation invariant solution, then* (34) *reduces to* (44) *in the thermodynamic limit.*

The idea of the proof is quite straightforward. Equation (34) is very similar to (44), but for the addition of the extra term $\bar R_2$. An inspection of (41) shows that the terms in $\bar R_2$ are mostly of the form $f-\langle f\rangle$, which vanish in the translation invariant case, and terms involving ϖ, which is set to 0 in the translation invariant case. The only remaining extra term is $\bar C(x)+\bar C(y)$, which we will show vanishes in the translation invariant case due to the identity (30).

Theorem 1 is quite general, and can be used to study a trapped Bose gas, in which there is an external potential v_0. In this case, ϖ is a multiplication operator by v_0. A natural approach is to scale v_0 with the volume: $v_0(x) = \bar{v}_0(V^{-1/3}x)$ in such a way that the size of the trap grows as $V \to \infty$, thus ensuring a finite local density in the thermodynamic limit. Following the ideas of Gross and Pitaevskii [18, 33], we would then expect to find that (33) and (34) decouple, and that (34) reduces to the translation invariant Eq. (44), with a density that is modulated over the trap. However, the presence of $\bar{R}_2$ in (34) and $\bar{C}$ in (33) breaks this picture. Further investigation of this question is warranted.

2.2 The Momentum Distribution

The momentum distribution for the Bose gas is defined as

$$\mathcal{M}^{(\text{Exact})}(k) := \frac{1}{N}\sum_{i=1}^{N}\langle\varphi_0|\, P_i\, |\varphi_0\rangle \tag{47}$$

where φ_0 is the ground state of the Hamiltonian

$$-\frac{1}{2}\sum_{i=1}^{N}\Delta_i + \sum_{1\leqslant i<j\leqslant N} v(x_i - x_j) \tag{48}$$

and

$$\varpi f := \epsilon|e^{ikx}\rangle\langle e^{ikx}|f \equiv \epsilon e^{ikx}\int dy\; e^{-iky} f(y) \tag{49}$$

and P_i is defined as in (2):

$$P_i\psi(x_1,\dots,x_N) = \epsilon e^{ikx_i}\int dy_y\; e^{iky_i}\psi(x_1,\dots,x_{i-1},y_i,x_{i+1},\dots,x_N). \tag{50}$$

Equivalently,

$$\mathcal{M}^{(\text{Exact})}(k) = \frac{\partial}{\partial\epsilon}\frac{E_0}{N}\bigg|_{\epsilon=0} \tag{51}$$

where E_0 is the ground-state energy in (4) for the Hamiltonian (48). Using the simplified approach, we do not have access to the ground state wavefunction, so we cannot compute $\mathcal{M}$ using (47). Instead, we use the Hellmann-Feynman theorem, which consists in adding $\sum_i P_i$ to the Hamiltonian. However, doing so does not ensure the uniqueness of the ground state, and thus, we are not guaranteed that the wavefunction ψ_0 is translation invariant. This is why Theorem 1 is needed to compute the momentum distribution within the framework of the Simplified approach. (A similar computation was done in [10], but, there, the derivation of the momentum distribution for the Simplified approach was taken for granted.)

By Theorem 1, and, in particular, (43), we obtain a natural definition of the prediction of the Simplified approach for the momentum distribution:

$$\mathcal{M}(k) := \frac{\partial}{\partial\epsilon}\left(\langle\mathcal{E}\rangle + \langle\varpi\rangle\right)|_{\epsilon=0}\,. \tag{52}$$

Theorem 2 (Momentum distribution) *Under the assumptions of Theorem 1, using periodic boundary conditions, if v is translation invariant and $\varpi = 0$, and if (33) and (34) have* *solutions that are twice differentiable in* ϵ*, uniformly in* V*, then, if* $k \neq 0$*,*

$$\mathcal{M}(k) = \frac{\partial}{\partial \epsilon} \frac{\rho}{2} \int dx\ (1 - u(x))v(x) \Big|_{\epsilon=0} \tag{53}$$

where

$$-\Delta u(x) = (1 - u(x))v(x) - 2\rho K(x) + \rho^2 L(x) + \epsilon F(x) \tag{54}$$

where K *and* L *are those of the translation invariant Simplified approach* (45) *and* (46) *and*

$$F(x) := -2\hat{u}(-k)\cos(kx). \tag{55}$$

We thus compute the momentum distribution. To check that our prediction is plausible, we compare it to the Bogolyubov prediction, which can easily be derived from [29, Appendix A]:

$$\mathcal{M}^{(\text{Bogolyubov})}(k) = -\frac{1}{2\rho}\left(1 - \frac{k^2 + 2\rho\hat{v}(k)}{\sqrt{k^4 + 4k^2\rho\hat{v}(k)}}\right) \tag{56}$$

(this can be obtained by differentiating [29, (A.26)] with respect to $\epsilon(k)$, which returns the number of particles in the state e^{ikx}, which we divide by ρ to obtain the momentum distribution). Actually, following the ideas of [23], we replace $\hat{v}$ by a so-called "pseudopotential", which consists in replacing v by a Dirac delta function, while preserving the scattering length:

$$\hat{v}(k) = 4\pi a \tag{57}$$

where the scattering length a is defined in [29, Appendix C]. Thus,

$$\mathcal{M}^{(\text{Bogolyubov})}(k) = -\frac{1}{2\rho}\left(1 - \frac{k^2 + 8\pi\rho a}{\sqrt{k^4 + 16\pi k^2\rho a}}\right). \tag{58}$$

We prove that, for the simple equation, as $\rho \to 0$, the prediction for the momentum distribution coincides with Bogolyubov's, for $|k| \lesssim \sqrt{\rho a}$. The length scale $1/\sqrt{\rho a}$ is called the *healing length*, and is the distance at which pairs of particles correlate [15]. It is reasonable to expect the Bogolyubov approximation to break down beyond this length scale.

The momentum distribution for the simple equation, following the prescription detailed in [8–10, 20], is defined as

$$\mathcal{M}^{(\text{simpleq})}(k) = \frac{\partial}{\partial \epsilon} \frac{\rho}{2} \int dx\ (1 - u(x))v(x) \Big|_{\epsilon=0} \tag{59}$$

where [8, (1.1)–(1.2)]

$$-\Delta u(x) = (1 - u(x))v(x) - 4eu + 2\rho e u * u + \epsilon F(x), \quad e := \frac{\rho}{2}\int dx\ (1 - u(x))v(x) \tag{60}$$

where F was defined in (55).

Theorem 3 *Assume that* v *is translation and rotation invariant* ($v(x, y) \equiv v(|x - y|)$)*, and consider periodic boundary conditions. We rescale* k*:*

$$\kappa := \frac{k}{2\sqrt{e}} \tag{61}$$

we have, for all $\kappa \in \mathbb{R}^3$*,*

$$\lim_{e\to 0}\rho\mathcal{M}^{(\text{simpleq})}(2\sqrt{e}\kappa)=\lim_{e\to 0}\rho\mathcal{M}^{(\text{Bogolyubov})}(2\sqrt{e}\kappa)=-\frac{1}{2}\left(1-\frac{\kappa^2+1}{\sqrt{(\kappa^2+1)^2-1}}\right). \quad (62)$$

The rotation invariance of v is presumably not necessary. However, the proof of this theorem is based on [9], where rotational symmetry was assumed for convenience.

3 The Simplified Approach Without Translation Invariance, Proof of Theorem 1

3.1 Factorization

We will first compute f_i and u_i for $i=3,4$ in Assumption 1.

3.1.1 Factorization of g_3

Lemma 1 *Assumption* 1 *with* $i=2,3$ *and* (29)–(31) *imply that*

$$g_3(x,y,z)=g_1(x)g_1(y)g_1(z)(1-u_3(x,y))(1-u_3(x,z))(1-u_3(y,z))(1+O(V^{-2})) \quad (63)$$

with

$$u_3(x,y):=u_2(x,y)+\frac{w_3(x,y)}{V} \quad (64)$$

$$w_3(x,y):=(1-u_2(x,y))\int dz\; g_1(z)u_2(x,z)u_2(y,z). \quad (65)$$

Proof Using (31) in (25),

$$g_2(x_1,x_2)=W_3(x_1,x_2)\int\frac{dx_3}{V}\;W_3(x_1,x_3)W_3(x_2,x_3). \quad (66)$$

1. We first expand to order V^{-1}. By (27),

$$\int\frac{dz}{V}\,f_3^2(z)u_3(x,z)=O(V^{-1}) \quad (67)$$

so, by (26),

$$g_2(x,y)=f_3^2(x)f_3^2(y)(1-u_3(x,y))\left(\int\frac{dz}{V}\;f_3^2(z)+O(V^{-1})\right). \quad (68)$$

By (24),

$$g_1(x)g_1(y)(1-u_2(x,y))=f_3^2(x)f_3^2(y)(1-u_3(x,y))\left(\int\frac{dz}{V}\;f_3^2(z)+O(V^{-1})\right). \quad (69)$$

We take $\int\frac{dy}{V}\cdot$ on both sides of this equation. However, by (30),

$$g_1(x)\int\frac{dy}{V}\;g_1(y)(1-u_2(x,y))=g_1(x) \quad (70)$$

so, by (29),

$$\int dy\; g_1(y)u_2(x,y) = 0. \tag{71}$$

Combining this with (67), we find

$$g_1(x) = f_3^2(x)\left(\left(\int \frac{dy}{V} f_3^2(y)\right)^2 + O(V^{-1})\right) \tag{72}$$

and, integrating once more implies that $\int \frac{dy}{V} f_3^2(y) = 1 + O(V^{-1})$. Therefore,

$$f_3^2(x) = g_1(x)(1 + O(V^{-1})) \tag{73}$$

and

$$u_3(x,y) = u_2(x,y)(1 + O(V^{-1})). \tag{74}$$

2. We push the expansion to order V^{-2}: (66) is

$$g_2(x,y) = f_3^2(x) f_3^2(y)(1 - u_3(x,y)) \int \frac{dz}{V} f_3^2(z)\,(1 - u_3(x,z) - u_3(y,z) + u_3(x,z)u_3(y,z))\,. \tag{75}$$

By (73)–(74) and (24),

$$\begin{aligned} f_3^2(x) f_3^2(y)(1 - u_3(x,y)) \int \frac{dz}{V} f_3^2(z) &= g_1(x)g_1(y)(1 - u_2(x,y)) \\ \cdot \left(1 + \int \frac{dz}{V}\,(g_1(z)(u_2(x,z) + u_2(y,z) - u_2(x,z)u_2(y,z))) + O(V^{-2})\right)&. \end{aligned} \tag{76}$$

Therefore, by (71),

$$\begin{aligned} f_3^2(x) f_3^2(y)(1 - u_3(x,y)) \int \frac{dz}{V} f_3^2(z) &= g_1(x)g_1(y)(1 - u_2(x,y)) \\ \cdot \left(1 - \int \frac{dz}{V} g_1(z)u_2(x,z)u_2(y,z) + O(V^{-2})\right)&. \end{aligned} \tag{77}$$

Now, let us apply $\int \frac{dy}{V} \cdot$ to both sides of the equation. Note that, by (27),

$$\int \frac{dy}{V}\, g_1(y)u_2(x,y) \int \frac{dz}{V} g_1(z)u_2(x,z)u_2(y,z) = O(V^{-2}). \tag{78}$$

Furthermore, by (71),

$$\int \frac{dy}{V}\, g_1(y)u_2(x,y) = 0, \quad \int \frac{dy}{V}\, g_1(y) \int \frac{dz}{V}\, g_1(z)u_2(x,z)u_2(y,z) = 0 \tag{79}$$

and by (73) and (74),

$$\int \frac{dy}{V}\, f_3^2(y)u_3(x,y) = \int \frac{dy}{V}\, g_1(y)u_2(x,y) + O(V^{-2}) = O(V^{-2}). \tag{80}$$

We are thus left with

$$f_3^2(x)\left(\int \frac{dy}{V}\, f_3^2(y)\right)^2 = g_1(x)(1 + O(V^{-2})). \tag{81}$$

Taking $\int \frac{dx}{V}\cdot$, we thus find that

$$\left(\int \frac{dx}{V} f_3^2(x)\right)^3 = 1 + O(V^{-2}) \tag{82}$$

and

$$f_3^2(x) = g_1(x)(1 + O(V^{-2})). \tag{83}$$

Therefore,

$$1 - u_3(x,y) = (1 - u_2(x,y))\left(1 - \frac{1}{V}\int dz\ g_1(z)u_2(x,z)u_2(y,z) + O(V^{-2})\right). \tag{84}$$

□

3.1.2 Factorization of g_4

Lemma 2 *Assumption 1 and (29)–(32) imply that*

$$g_4(x_1,x_2,x_3,x_2) = g_1(x_1)g_1(x_2)g_1(x_3)g_1(x_4)\left(\prod_{i<j}(1 - u_4(x_i,x_j))\right)(1 + O(V^{-2})) \tag{85}$$

with

$$u_4(x,y) := u_2(x,y) + \frac{2w_3(x,y)}{V} \tag{86}$$

where w_3 is the same as in Lemma 1.

Proof Using (32) in (25),

$$g_2(x_1,x_2) = W_4(x_1,x_2)\int \frac{dx_3dx_4}{V^2}\ W_4(x_1,x_3)W_4(x_1,x_4)W_4(x_2,x_3)W_4(x_2,x_4)W_4(x_3,x_4). \tag{87}$$

1. We expand to order V^{-1}. By (27),

$$\int \frac{dz}{V} f_4^3(z)u_4(x,z) = O(V^{-1}) \tag{88}$$

so by (26),

$$g_2(x,y) = f_4^3(x)f_4^3(y)(1 - u_4(x,y))\left(\int \frac{dzdt}{V^2} f_4^3(z)f_4^3(t) + O(V^{-1})\right). \tag{89}$$

By (24),

$$g_1(x)g_1(y)(1 - u_2(x,y)) = f_4^3(x)f_4^3(y)(1 - u_4(x,y))\left(\left(\int \frac{dz}{V} f_4^3(z)\right)^2 + O(V^{-1})\right). \tag{90}$$

Applying $\int \frac{dy}{V}\cdot$ to both sides of the equation, using (71) and (88),

$$g_1(x) = f_4(x)^3\left(\left(\int \frac{dy}{V}\ f_4^3(y)\right)^3 + O(V^{-1})\right). \tag{91}$$

Integrating once more, we have $\int \frac{dy}{V} f_4^3(z) = 1 + O(V^{-1})$ and

$$f_4^3(x) = g_1(x)(1 + O(V^{-1})). \tag{92}$$

Therefore,

$$u_4(x, y) = u_2(x, y)(1 + O(V^{-1})). \tag{93}$$

2. We push the expansion to order V^{-2}: by (27),

$$\int \frac{dzdt}{V^2} u_4(x, z)u_4(y, t) = O(V^{-2}), \quad \int \frac{dzdt}{V^2} u_4(x, z)u_4(z, t) = O(V^{-2}) \tag{94}$$

$$\int \frac{dzdt}{V^2} u_4(x, z)u_4(x, t) = O(V^{-2}) \tag{95}$$

so

$$g_2(x, y) = f_4^3(x) f_4^3(y)(1 - u_4(x, y)) \left(\int \frac{dzdt}{V^2} f_4^3(z) f_4^3(t) \right.$$
$$\left. + \int \frac{dzdt}{V^2} g_1(z)g_1(t)(-2u_4(x, z) - 2u_4(y, z) - u_4(z, t) + 2u_4(x, z)u_4(y, z)) + O(V^{-2}) \right). \tag{96}$$

By (92), (93), and (24)

$$f_4^3(x) f_4^3(x)(1 - u_4(x, y)) \left(\int \frac{dz}{V} f_4^3(z) \right)^2 = g_1(x)g_1(y)(1 - u_2(x, y))$$
$$\cdot \left(1 + \int \frac{dzdt}{V^2} g_1(z)g_1(t)(2u_2(x, z) + 2u_2(y, z) + u_2(z, t) - 2u_2(x, z)u_2(y, z)) + O(V^{-2}) \right). \tag{97}$$

By (71),

$$f_4^3(x) f_4^3(y)(1 - u_4(x, y)) \left(\int \frac{dz}{V} f_4^3(z) \right)^2$$
$$= g_1(x)g_1(y)(1 - u_2(x, y)) \left(1 - 2 \int \frac{dz}{V} g_1(z)u_2(x, z)u_2(y, z) + O(V^{-2}) \right). \tag{98}$$

We apply $\int \frac{dy}{V} \cdot$ to both sides of the equation. By (78)-(80), we find

$$f_4^3(x) \left(\int \frac{dy}{V} f_4^3(z) \right)^3 = g_1(x)(1 + O(V^{-2})). \tag{99}$$

Taking $\int \frac{dx}{V} \cdot$, we find that

$$f_4(x) = 1 + O(V^{-2}) \tag{100}$$

and

$$f_4^3(x) = g_1(x)(1 + O(V^{-2})). \tag{101}$$

Therefore,

$$1 - u_4(x, y) = (1 - u_2(x, y)) \left(1 - \frac{2}{V} \int dz \, g_1(z)u_2(x, z)u_2(y, z) + O(V^{-2}) \right). \tag{102}$$

□

3.2 Consequences of the Factorization

proof of Theorem 1 We rewrite (10), (14) and (19) using Lemmas 1 and 2.

1. We start with (10): by (5) and (24),

$$G_0^{(2)} = \frac{N(N-1)}{2V^2} \int dxdy\; v(x,y)g_1(x)g_1(y)(1-u_2(x,y)) + O(V^{-1}) \tag{103}$$

so

$$E_0 = \frac{N(N-1)}{2V^2} \int dxdy\; v(x,y)g_1(x)g_1(y)(1-u_2(x,y)) \\ + \frac{N}{V}\int dx\; \varpi g_1(x) + B_0 + O(V^{-1}). \tag{104}$$

2. We now turn to (14): by (5) and (24),

$$G_1^{(2)}(x) = \frac{N}{V} g_1(x) \left(\int dy\; v(x,y)g_1(y)(1-u_2(x,y)) + O(V^{-2}) \right) \tag{105}$$

and by Lemma 1,

$$G_1^{(3)}(x) = g_1(x) \left(\frac{N^2}{2V^2} \int dydz\; v(y,z)g_1(y)g_1(z)(1-u_2(x,y))(1-u_2(x,z)) \right. \\ \left. (1-u_3(y,z)) - \frac{3N}{2V^2} \int dydz\; v(y,z)g_1(y)g_1(z)(1-u_2(y,z)) + O(V^{-1}) \right) \tag{106}$$

(we used (64) to write $u_3 = u_2 + O(V^{-1})$; this works fine for $u_3(x,y)$ and $u_3(x,z)$ because the integrals over y and z are controlled by $v(y,z)w_3(x,y)$ and $v(y,z)w_3(x,z)$ using (5) and (27); in the first term, it does not work for $u_3(y,z)$, as $v(y,z)w_3(y,z)$ can only control one of the integrals, and not both; the second term has an extra V^{-1} that lets us replace u_3 by u_2) and by (27) and (6),

$$F_1^{(2)}(x) = g_1(x) \left(\frac{N}{V} \int dy\; \varpi_y (g_1(y)(1-u_2(x,y))) - \frac{1}{V} \int dy\; \varpi g_1(y) + O(V^{-1}) \right). \tag{107}$$

The first term in $G_1^{(3)}$ is of order V:

$$\frac{N^2}{2V^2} \int dydz\; v(y,z)g_1(y)g_1(z)(1-u_2(x,y))(1-u_2(x,z))(1-u_3(y,z)) \\ = \frac{N^2}{2V^2} \int dydz\; v(y,z)g_1(y)g_1(z)(1-u_2(y,z)) \\ - \frac{N^2}{2V^3} \int dydz\; v(y,z)g_1(y)g_1(z)w_3(y,z) + \\ + \frac{N^2}{2V^2} \int dydz\; v(y,z)g_1(y)g_1(z)(1-u_2(y,z))(-u_2(x,y) \\ -u_2(x,z) + u_2(x,y)u_2(x,z)) + O(V^{-1}) \tag{108}$$

in which the only term of order V is the first one, and is equal to the first term of order V in E_0, and thus cancels out. There is a similar cancellation between the second term of order V in $F_1^{(2)}$ and E_0. All in all,

$$\left(-\frac{\Delta}{2}+\varpi+\bar G_1^{(2)}(x)+\bar G_1^{(3)}(x)+\bar F_1^{(2)}(x)+\bar E_0-B_0\right)g_1(x)+B_1(x)=g_1(x)O(V^{-1}) \quad (109)$$

with, recalling $\rho := N/V$,

$$\bar G_1^{(2)}(x) := \rho\int dy\ v(x,y)g_1(y)(1-u_2(x,y)) \quad (110)$$

and using (65),

$$\begin{aligned}\bar G_1^{(3)}(x) &:= -\frac{\rho}{2}\int\frac{dydz}{V}\ v(y,z)g_1(y)g_1(z)(1-u_2(y,z))\left(3+\rho\int dt\ g_1(t)u_2(y,t)u_2(z,t)\right)+\\ &\quad+\frac{\rho^2}{2}\int dydz\ v(y,z)g_1(y)g_1(z)(1-u_2(y,z))(-u_2(x,y)-u_2(x,z)+u_2(x,y)u_2(x,z)) \quad (111)\\ \bar F_1^{(2)}(x) &:= -\rho\int dy\ \varpi_y(g_1(y)u_2(x,y))-\int\frac{dy}{V}\ \varpi g_1(y) \quad (112)\\ \bar E_0 &:= \frac{\rho}{2}\int\frac{dxdy}{V}\ v(x,y)g_1(x)g_1(y)(1-u_2(x,y)). \quad (113)\end{aligned}$$

Rewriting this using (35)–(38), we find (33) with

$$\Sigma_1(x) := B_1(x)-B_0g_1(x)+O(V^{-1}). \quad (114)$$

3. Finally, we rewrite (19): by (5) and Lemma 1,

$$\begin{aligned}G_2^{(3)}(x,y) &= \frac{N}{V}g_1(x)g_1(y)(1-u_2(x,y))\\ &\quad\cdot\left(\int dz\ (v(x,z)+v(y,z))g_1(z)(1-u_2(x,z))(1-u_2(y,z))+O(V^{-1})\right) \quad (115)\end{aligned}$$

and by Lemma 2,

$$\begin{aligned}G_2^{(4)}(x,y) &= g_1(x)g_1(y)\left(\frac{N^2}{2V^2}(1-u_4(x,y))\right.\\ &\quad\int dzdt\ v(z,t)g_1(z)g_1(t)(1-u_4(z,t))\Pi(x,y,z,t)\\ &\quad\left.-\frac{5N}{2V^2}(1-u_2(x,y))\int dzdt\ v(z,t)g_1(z)g_1(t)(1-u_2(z,t))+O(V^{-1})\right) \quad (116)\\ \Pi(x,y,z,t) &:= (1-u_2(x,z))(1-u_2(x,t))(1-u_2(y,z))(1-u_2(y,t)) \quad (117)\end{aligned}$$

and by (27) and (6),

$$\begin{aligned}F_2^{(3)}(x,y) &= g_1(x)g_1(y)\left(\frac{N}{V}(1-u_3(x,y))\int dz\ \varpi_z(g_1(z)(1-u_2(x,z))(1-u_2(y,z)))\right.\\ &\quad\left.-\frac{2}{V}(1-u_2(x,y))\int dz\ \varpi g_1(z)+O(V^{-1})\right). \quad (118)\end{aligned}$$

The first term in $G_2^{(4)}$ is of order V: by (86),

$$\begin{aligned}
&\frac{N^2}{2V^2}(1-u_4(x,y))\int dzdt\ v(z,t)g_1(z)g_1(t)(1-u_4(z,t))\Pi(x,y,z,y)\\
&=\frac{N^2}{2V^2}(1-u_2(x,y))\int dzdt\ v(z,t)g_1(z)g_1(t)(1-u_2(z,t))\\
&-\frac{N^2}{V^3}w_3(x,y)\int dzdt\ v(z,t)g_1(z)g_1(y)(1-u_2(z,t))\\
&-\frac{N^2}{V^3}(1-u_2(x,y))\int dzdt\ v(z,t)g_1(z)g_1(t)w_3(z,t)\\
&+\frac{N^2}{2V^2}(1-u_2(x,y))\int dzdt\ v(z,t)g_1(z)g_1(t)(1-u_2(z,t))\,(\Pi(x,y,z,t)-1)+O(V^{-1})
\end{aligned}\tag{119}$$

in which the only term of order V is the first one, and is equal to the term of order V in E_0, and thus cancels out. There is a similar cancellation between the term of order V in $F_2^{(3)}$ and E_0. All in all,

$$\begin{aligned}
&\left(-\frac{1}{2}(\Delta_x+\Delta_y)+v(x,y)+\varpi_x+\varpi_y+\bar{G}_2^{(3)}(x,y)+\bar{G}_2^{(4)}(x,y)+\bar{F}_2^{(3)}(x,y)+\bar{E}_0-B_0\right)\\
&\cdot g_1(x)g_1(y)(1-u_2(x,y))+B_2(x,y)=g_1(x)g_1(y)O(V^{-1})
\end{aligned}\tag{120}$$

with

$$\bar{G}_2^{(3)}(x,y):=\rho\int dz\ (v(x,z)+v(y,z))g_1(z)(1-u_2(x,z))(1-u_2(y,z))\tag{121}$$

and by (65),

$$\begin{aligned}
\bar{G}_2^{(4)}(x,y):=&-\frac{\rho}{2}\left(5+2\rho\int dr\ g_1(r)u_2(x,r)u_2(y,r)\right)\\
&\int\frac{dzdt}{V}\ v(z,t)g_1(z)g_1(t)(1-u_2(z,t))-\\
&-\rho^2\int\frac{dzdt}{V}\ v(z,t)g_1(z)g_1(t)(1-u_2(z,t))\int dr\ g_1(r)u_2(z,r)u_2(t,r)+\\
&+\frac{\rho^2}{2}\int dzdt\ v(z,t)g_1(z)g_1(t)(1-u_2(z,t))\,(\Pi(x,y,z,t)-1)
\end{aligned}\tag{122}$$

$$\begin{aligned}
\bar{F}_2^{(3)}(x,y)\ &:=\rho\int dz\ \varpi_z(g_1(z)(-u_2(x,z)-u_2(y,z)+u_2(x,z)u_2(y,z)))\\
&-\left(2+\rho\int dr\ g_1(r)u_2(x,r)u_2(y,r)\right)\int\frac{dz}{V}\ \varpi g_1(z)
\end{aligned}\tag{123}$$

$$\bar{E}_0\ =\frac{\rho}{2}\int\frac{dxdy}{V}\ v(x,y)g_1(x)g_1(y)(1-u_2(x,y)).\tag{124}$$

4. Expanding out Π, see (117), we find (34) with

$$\begin{aligned}
\bar{R}_2(x,y):=\rho&\int dz\ g_1(z)\left(\bar{S}(x,z)+\bar{S}(y,z)-2\int\frac{dt}{V}\ g_1(t)\bar{S}(t,z)\right)\\
&+\frac{\rho^2}{2}\left(\bar{S}\bar{*}u_2\bar{*}u_2(x,x)+\bar{S}\bar{*}u_2\bar{*}u_2(y,y)-2\int\frac{dt}{V}\ g_1(t)\bar{S}\bar{*}u_2\bar{*}u_2(t,t)\right)\\
&+\rho^2\int dzdt\ g_1(z)g_1(t)u_2(x,z)u_2(y,z)\left(\bar{S}(z,t)-\int\frac{dr}{V}\ g_1(r)\bar{S}(z,r)\right)\\
&-\rho^2\int dt\ g_1(t)(\bar{S}\bar{*}u_2(x,t)+\bar{S}\bar{*}u_2(y,t))+\bar{F}_2^{(3)}(x,y)+\varpi_x+\varpi_y
\end{aligned}\tag{125}$$

and

$$\Sigma_2(x,y):=B_2(x,y)-B_0g_1(x)g_1(y)(1-u_2(x,y))+O(V^{-1}).\tag{126}$$

Using (37) and (38), (125) becomes (41).

5. Finally, (43) follows from (10) with

$$\Sigma_0 := B_0 + O(V^{-1}). \tag{127}$$

□

3.3 Sanity Check, Proof of Corollary 1

Proof of Corollary 1 Assuming the translation invariance of the solution, $g_1(x)$ is constant. By (29),

$$g_1(x) = 1. \tag{128}$$

Furthermore, $\varpi \equiv 0$. We then have

$$\bar{S}(x, y) = S(x - y), \quad \bar{K}(x, y) = K(x - y), \quad \bar{L}(x, y) = L(x - y) \tag{129}$$

(see (45) and (46)). Furthermore,

$$\mathcal{E}(x) \equiv \mathcal{E}(y) \equiv \langle \mathcal{E} \rangle = \frac{\rho}{2} \int dy\; S(y) \tag{130}$$

$$\bar{A}(x) \equiv \bar{A}(y) \equiv \langle \bar{A} \rangle = \rho^2 S * u * u(0) \tag{131}$$

$$\bar{C}(x) \equiv \bar{C}_2(y) = 2\rho^2 \int dz\; u(z) \int dt\; S(t) \tag{132}$$

which vanishes by (30). Thus,

$$\bar{R}_2(x, y) \equiv 0. \tag{133}$$

We conclude by taking the thermodynamic limit.

4 The Momentum Distribution

4.1 Computation of the Momentum Distribution, Proof of Theorem 2

Proof of Theorem 2 We use Theorem 1 with ϖ as in (49). Note that, by (49),

$$\int dx\; \varpi f(x) = 0 \tag{134}$$

which trivially satisfies (6).

1. We change variables in (34) to

$$\xi = \frac{x + y}{2}, \quad \zeta = x - y \tag{135}$$

and find

$$\left(-\frac{1}{4}\Delta_\xi - \Delta_\zeta + v(\zeta) - 2\rho\bar{K}(\xi + \tfrac{\zeta}{2}, \xi - \tfrac{\zeta}{2}) + \rho^2\bar{L}(\xi + \tfrac{\zeta}{2}, \xi - \tfrac{\zeta}{2}) + \bar{R}_2(\xi + \tfrac{\zeta}{2}, \xi - \tfrac{\zeta}{2})\right)$$
$$\cdot g_1(\xi + \tfrac{\zeta}{2}) g_1(\xi - \tfrac{\zeta}{2})(1 - u_2(\xi + \tfrac{\zeta}{2}, \xi - \tfrac{\zeta}{2})) = -\Sigma_2. \tag{136}$$

In addition, by (43),

$$e=\frac{\rho}{2}\int\frac{d\xi d\zeta}{V}\;g_1(\xi+\tfrac{\zeta}{2})g_1(\xi-\tfrac{\zeta}{2})v(\zeta)(1-u_2(\xi+\tfrac{\zeta}{2},\xi-\tfrac{\zeta}{2}))+\int\frac{dx}{V}\;\varpi g_1(x)+\Sigma_1. \quad (137)$$

We expand in powers of ϵ:

$$g_1(x)=1+\epsilon g_1^{(1)}(x)+O(\epsilon^2),\quad u_2(\xi+\tfrac{\zeta}{2},\xi-\tfrac{\zeta}{2})=u_2^{(0)}(\zeta)+\epsilon u_2^{(1)}(\xi+\tfrac{\zeta}{2},\xi-\tfrac{\zeta}{2})+O(\epsilon^2) \quad (138)$$

in which we used the fact that, at $\epsilon=0$, $g_1(x)|_{\epsilon=0}=1$, see (128). In particular, the terms of order 0 in ϵ are independent of ξ. Note, in addition, that, by (29),

$$\int\frac{dx}{V}\;g_1^{(1)}(x)=0. \quad (139)$$

2. The trick of this proof is to take the average with respect to ξ on both sides of (136). Since we take periodic boundary conditions, the Δ_ξ term drops out. We will only focus on the first order contribution in ϵ, and, as was mentioned above, terms of order 0 are independent of ξ. Thus, the average over ξ will always apply to a single term, either $g_1^{(1)}$ or $u_2^{(1)}$. By (29), the terms involving $g_1^{(1)}$ have zero average. We can therefore replace $g_1^{(1)}$ by 1. (The previous argument does not apply to the terms in which Δ_ζ acts on g_1, but these terms have a vanishing average as well because of the periodic boundary conditions.) In particular, by (30) and (24),

$$\int\frac{d\xi}{V}\;(1-u_2^{(1)}(\xi+\tfrac{\zeta}{2},\xi-\tfrac{\zeta}{2}))=1 \quad (140)$$

so

$$\int\frac{d\xi}{V}\;u_2^{(1)}(\xi+\tfrac{\zeta}{2},\xi-\tfrac{\zeta}{2})=0 \quad (141)$$

and thus, we can replace u_2 with $u_2^{(0)}$. Thus, using the translation invariant computation detailed in Sect. 3.3, we find that the average of (136) is

$$(-\Delta+v(\zeta)-2\rho K(\zeta)+\rho^2L(\zeta))(1-u_2^{(0)}(\zeta))+\epsilon F(\zeta)+O(\epsilon^2)+\Sigma_2=0 \quad (142)$$

where K and L are defined in (45) and (46) and F comes from the contribution to $\bar R_2$ of ϖ, see (41):

$$\begin{aligned}F(\zeta)\;&:=\epsilon^{-1}\int\frac{d\xi}{V}\;\Big(\varpi_x+\varpi_y-2\langle\varpi\rangle+\rho\int dz\;\varpi_z(u_2^{(0)}(\xi+\tfrac{\zeta}{2}-z)u_2^{(0)}(\xi-\tfrac{\zeta}{2}-z))\\&\quad-\rho\int dz\;\varpi_z u_2^{(0)}(\xi+\tfrac{\zeta}{2}-z)-\rho\int dz\;\varpi_z u_2^{(0)}(\xi-\tfrac{\zeta}{2}-z)\Big)\,(1-u_2^{(0)}(\zeta)). \quad (143)\end{aligned}$$

Similarly, (137) is

$$e=\frac{\rho}{2}\int d\zeta\;v(\zeta)(1-u_2^{(0)}(\zeta))+\int\frac{dx}{V}\;\varpi g_1(x)+\Sigma_1+O(\epsilon^2). \quad (144)$$

3. Furthermore, by (49),

$$\int dz\;\varpi_z f(z)=0 \quad (145)$$

for any integrable f, so

$$F(\zeta)=\epsilon^{-1}\int\frac{d\xi}{V}\;\left(\varpi_x+\varpi_y\right)(1-u_2^{(0)}(\zeta)) \quad (146)$$

and

$$e=\frac{\rho}{2}\int d\zeta\ v(\zeta)(1-u_2^{(0)}(\zeta))+\Sigma_1+O(\epsilon^2). \tag{147}$$

Now,

$$\varpi_x f(x-y)=e^{ikx}\int dz\ e^{-ikz}f(z-y) \tag{148}$$

so

$$\varpi_x f(\zeta)=\epsilon e^{ik(\xi+\frac{\zeta}{2})}\int dz\ e^{-ik(z+(\xi-\frac{\zeta}{2}))}f(z)=\epsilon e^{ik\zeta}\int dz\ e^{-ikz}f(z)=\epsilon e^{ik\zeta}\hat f(-k). \tag{149}$$

Similarly,

$$\varpi_y f(\zeta)=\epsilon e^{-ik\zeta}\hat f(-k). \tag{150}$$

Thus

$$F(\zeta)=2\cos(k\zeta)(\delta(k)-\hat u_2^{(0)}(-k)). \tag{151}$$

Since $k\neq 0$, the δ function drops out. We conclude the proof by combining (142), (147) and (151) and taking the thermodynamic limit.

4.2 The Simple Equation and Bogolyubov Theory, Proof of Theorem 3

Proof of Theorem 3 1. We differentiate (60) with respect to ϵ and take $\epsilon=0$:

$$(-\Delta+v+4e+4e\rho u*)\partial_\epsilon u=-4\partial_\epsilon eu+2\partial_\epsilon e\rho u*u+F. \tag{152}$$

Let

$$\mathfrak{K}_e:=(-\Delta+v+4e(1-\rho u*))^{-1} \tag{153}$$

(this operator was introduced and studied in detail in [9]). We apply $\mathfrak{K}_e$ to both sides and take a scalar product with $-\rho v/2$ and find

$$\partial_\epsilon e=\rho\partial_\epsilon e\int dx\ v(x)\mathfrak{K}_e(2u(x)-\rho u*u(x))-\frac{\rho}{2}\int dx\ v(x)\mathfrak{K}_eF(x) \tag{154}$$

and so, using (59),

$$\mathcal{M}^{(\text{simpleq})}(k)=\partial_\epsilon e=-\frac{\frac{\rho}{2}\int dx\ v(x)\mathfrak{K}_eF(x)}{1-\rho\int dx\ v(x)\mathfrak{K}_e(2u(x)-\rho u*u(x))} \tag{155}$$

and, by (55),

$$\mathcal{M}^{(\text{simpleq})}(k)=\rho\frac{\hat u(k)\int dx\ v(x)\mathfrak{K}_e\cos(kx)}{1-\rho\int dx\ v(x)\mathfrak{K}_e(2u(x)-\rho u*u(x))}. \tag{156}$$

Note that

$$\int\frac{dk}{(2\pi)^3}\mathcal{M}^{(\text{simpleq})}(k)=\frac{\rho\int dx\ v(x)\mathfrak{K}_eu(x)}{1-\rho\int dx\ v(x)\mathfrak{K}_e(2u(x)-\rho u*u(x))} \tag{157}$$

which is the expression for the uncondensed fraction for the simple equation [10, (38)].

2. By [9, (5.8), (5.27)],

$$\mathcal{M}^{(\text{simpleq})}(k) = \rho\left(\hat{u}(k)\int dx\; v(x)\mathfrak{K}_e\cos(k(x))\right)(1 + O(\rho e^{-\frac{1}{2}})). \tag{158}$$

Furthermore, by the resolvent identity,

$$\mathfrak{K}_e\cos(kx) = \xi - \mathfrak{K}_e(v\xi),\quad \xi := \mathfrak{Y}_e(\cos(kx)) := (-\Delta + 4e(1-\rho u*))^{-1}\cos(kx) \tag{159}$$

in terms of which, using the self-adjointness of $\mathfrak{K}_e$,

$$\mathcal{M}^{(\text{simpleq})}(k) = \rho\hat{u}(k)\left(\int dx\; v(x)\xi(x) - \int dx\; \mathfrak{K}_e v(x)(v(x)\xi(x))\right). \tag{160}$$

3. Now, taking the Fourier transform,

$$\hat{\xi}(q) \equiv \int dx\; e^{ikx}\xi(x) = \frac{(2\pi)^3}{2}\frac{\delta(k-q)+\delta(k+q)}{q^2+4e(1-\rho\hat{u}(q))} \tag{161}$$

and so

$$\int dx\; v(x)\xi(x) = \int \frac{dq}{(2\pi)^3}\hat{v}(q)\hat{\xi}(q) = \frac{\hat{v}(k)}{k^2+4e(1-\rho\hat{u}(k))} \tag{162}$$

and thus

$$\rho\hat{u}(k)\int dx\; v(x)\xi = \rho\hat{v}(k)\frac{\hat{u}(k)}{k^2+4e(1-\rho\hat{u}(k))}. \tag{163}$$

We recall [8, (4.25)]:

$$\rho\hat{u}(k) = \frac{k^2}{4e} + 1 - \sqrt{\left(\frac{k^2}{4e}+1\right)^2 - \hat{S}(k)} \tag{164}$$

and, by [8, (4.24)],

$$\hat{S}(0) = 1. \tag{165}$$

Therefore, if we rescale

$$k = 2\sqrt{e}\kappa \tag{166}$$

we find

$$\rho\hat{u}(k)\int dx\; v(x)\xi = \frac{\hat{v}(0)}{4e}\frac{\kappa^2+1-\sqrt{(\kappa^2+1)^2-1}}{\sqrt{(\kappa^2+1)^2-1}} + o(e^{-1}). \tag{167}$$

4. Now,

$$\int dx\; e^{iqx}v(x)\xi(x) = \frac{1}{2}\frac{1}{k^2+4e(1-\rho\hat{u}(k))}\int dp\; \hat{v}(q-p)(\delta(k-p)+\delta(k+p)) \tag{168}$$

so

$$\int dx\; e^{iqx}v(x)\xi(x) = \frac{1}{2}\frac{\hat{v}(q-k)+\hat{v}(q+k)}{k^2+4e(1-\rho\hat{u}(k))}. \tag{169}$$

Therefore,

$$\int dx\ \mathfrak{K}_e v(x)(v\xi) = \frac{1}{2}\frac{1}{k^2+4e(1-\rho\hat u(k))}\int\frac{dq}{(2\pi)^3}\widehat{\mathfrak{K}_e v}(q)(\hat v(k-q)+\hat v(k+q)) \tag{170}$$

which, using the $q \mapsto -q$ symmetry, is

$$\int dx\ \mathfrak{K}_e v(x)(v\xi) = \frac{1}{k^2+4e(1-\rho\hat u(k))}\int\frac{dq}{(2\pi)^3}\widehat{\mathfrak{K}_e v}(q)\hat v(k+q) \tag{171}$$

that is,

$$\rho\hat u(k)\int dx\ \mathfrak{K}_e v(x)(v\xi) = \frac{\rho\hat u(k)}{k^2+4e(1-\rho\hat u(k))}\int dx\ e^{-ikx}\mathfrak{K}_e v(x)v(x) \tag{172}$$

in which we rescale

$$k = 2\sqrt{e}\kappa \tag{173}$$

so, by (164)-(165),

$$\rho\hat u(k)\int dx\ \mathfrak{K}_e v(x)(v\xi) = \frac{\kappa^2+1-\sqrt{(\kappa^2+1)^2-1}}{4e\sqrt{(\kappa^2+1)^2-1}}(1+o(1))\int dx\ e^{-i2\sqrt{e}\kappa x}v(x)\mathfrak{K}_e v(x). \tag{174}$$

Therefore, by dominated convergence (using the argument above [9, (5.23)] and the fact that $\mathfrak{K}_e$ is positivity preserving), and by [9, (5.23)-(5.24)],

$$\rho\hat u(k)\int dx\ \mathfrak{K}_e v(x)(v\xi) = \frac{\kappa^2+1-\sqrt{(\kappa^2+1)^2-1}}{4e\sqrt{(\kappa^2+1)^2-1}}(-4\pi a+\hat v(0))+o(e^{-1}). \tag{175}$$

5. Inserting (167) and (175) into (160), we find

$$\mathcal{M}^{(\mathrm{simpleq})}(k) = \frac{\pi a}{e}\frac{\kappa^2+1-\sqrt{(\kappa^2+1)^2-1}}{\sqrt{(\kappa^2+1)^2-1}}+o(e^{-1}). \tag{176}$$

Finally, we recall [8, (1.23)]:

$$e = 2\pi\rho a(1+O(\sqrt{\rho})) \tag{177}$$

so

$$\mathcal{M}^{(\mathrm{simpleq})}(k) = \frac{1}{2}\frac{\kappa^2+1-\sqrt{(\kappa^2+1)^2-1}}{\sqrt{(\kappa^2+1)^2-1}}+o(e^{-1}). \tag{178}$$

6. Finally, by (58)

$$\mathcal{M}^{(\mathrm{Bogolyubov})}(2\sqrt{e}\kappa) = -\frac{1}{2\rho}\left(1-\frac{\frac{4e}{8\pi\rho a}\kappa^2+1}{\sqrt{\frac{e^2}{4\pi^2\rho^2a^2}\kappa^4+\frac{e}{\pi\rho a}\kappa^2}}\right) \tag{179}$$

so by (177),

$$\mathcal{M}^{(\mathrm{Bogolyubov})}(2\sqrt{e}\kappa) = -\frac{1}{2\rho}\left(1-\frac{\kappa^2+1}{\sqrt{\kappa^4+2\kappa^2}}\right). \tag{180}$$

This, together with (178), implies (62).

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