# Analysis of the Bogoliubov free energy functional

a variational description of a weakly-interacting Bose gas

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# Summary

In this thesis, we analyse a variational reformulation of the Bogoliubov approximation that is used to describe weakly-interacting translationally-invariant Bose gases. For the resulting model, the 'Bogoliubov free energy functional', we demonstrate existence of minimizers as well as the presence of a phase transition to Bose–Einstein condensation, and establish the phase diagram. We also give a calculation of the critical temperature assuming the gas is dilute, and find that it agrees with earlier numerical studies.

The thesis contains an introduction, a physical review paper outlining the main results and ideas, and two mathematical papers with detailed proofs.

# Resumé

I denne afhandling analyserer vi en variationel reformulering af Bogoliubov approksimationen, som beskriver svagt vekselvirkende translationsinvariante Bose gasser. I den resulterende model 'Bogoliubovs frie energi funktional', viser vi eksistens af minima og tilstedeværelse af en faseovergang til Bose–Einstein kondensation, og finder fasediagrammet. Vi beregner den kritiske temperatur hvis gassen har lav tæthed, og finder at den passer med eksisterende numeriske resultater.

Afhandlingen består af en introduktion, en fysisk oversigtsartikel som forklarer de vigtigste resultater og ideer, og to matematiske artikler med beviser.

# Contents

# Introduction

## 1 Context and basic question

Below 2.17K, helium-4 is truly magic: it can defy gravity and climb up walls, escape the confinement of a container, and provide an endlessly flowing fountain. Kapitsa, Allen and Misener discovered these remarkable properties in 1937, and this phenomenon is now known as *superfluidity.* Much earlier, in 1911, Kamerlingh Onnes had noticed that very cold mercury has no resistance, which was the first example of something called *superconductivity.*

A theoretical concept that would prove a vital ingredient in explanations of both superconductivity and superfluidity had been discovered in 1924/25 by Bose and Einstein. Their theory describes a class of particles called *bosons.* Many atoms, such as helium-4, are examples of bosons. Their defining features are that they are manifestly *indistinguishable* and that they have an inclination to cluster. Mathematically, this property is expressed by the invariance of the quantum mechanical state under permutation of the particles. Exchanging the particles in a two-particle state $\Psi$, for example, should leave that state invariant since the two particles are indistinguishable, and therefore the same, that is,

$$\Psi(1, 2) = \Psi(2, 1). \tag{1}$$

How does this symmetry lead to a tendency to cluster? Imagine that we have two *distinguishable* particles in a 2-level system with basis states $|0\rangle$ and $|1\rangle$. A basis for the state space of two such particles consists of $|00\rangle$ and $|11\rangle$, together with $|01\rangle$ and $|10\rangle$. Note that there are two configurations where the particles are in the same state, and two were they are in different states. When we impose the symmetry (1), the first two states are still allowed, but the latter two are not since $|01\rangle \neq |10\rangle$. To describe bosons, we have to replace these two by the single *symmetric* state $(|01\rangle + |10\rangle)/\sqrt{2}$. Now, there are two configurations where the particles are in the same state ($|00\rangle$ and $|11\rangle$), and only one where they are in different states ($(|01\rangle + |10\rangle)/\sqrt{2}$). Hence, at least at the level of the number of configurations, bosons are more likely to be in the same state than distinguishable particles.

This observation provided the starting point for a more complete analysis, which led to the discovery of *Bose–Einstein condensation (BEC)*—an extreme consequence of the bosonic tendency to cluster.

The first step in this analysis was made in 1924, when Bose worked out the implications of the symmetry (1) for large numbers of non-interacting bosons. In other words, he developed statistics for bosons. The set-up is as follows: consider $N$ non-interacting bosons, which means that the Hamiltonian describing the system is a sum of (identical) 1-particle Hamiltonians. To obtain a configuration of the $N$-body system, we simply need to know the 1-body energy levels and distribute the particles among them. The $N$-body ground state is obtained by putting all the particles in the lowest-energy state, but with increasing temperature we expect that particles will also typically occupy states with higher energy (see Figure 1).

Bose described what the typical configuration is, and how it depends on the temperature $T$. To describe his conclusions, we should briefly mention two different descriptions of statistical-mechanical systems. On the one hand, we can describe them in the *canonical ensemble*, which means that we have a fixed particle number $N$ and temperature $T$. On the other hand, we can also only fix $T$ and allow the number of particles to vary. The average particle number is then controlled by a parameter known as the chemical potential $\mu$. This description with fixed $\mu$ and $T$ is known as the *grand canonical ensemble.*

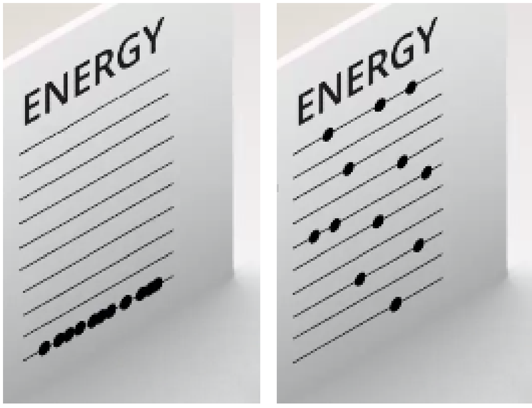


Figure 1: The ground (or zero temperature) state of a system of non-interacting bosons (left), and a possible configuration at higher temperatures (right). The 1-particle quantum states are schematically depicted by lines, ordered by energy from low to high. At zero temperature, all bosons are in the ground state of the 1-body Hamiltonian, whereas they spread out over higher and higher levels as the temperature increases.

Without commenting on the derivation, for a system with 1-particle eigenstates with energies $\epsilon_0 \leq \epsilon_1 \leq \dots$, the expected occupancy of the $j^{\text{th}}$ level is (setting $\hbar = 2m = k_B = 1$)

$$\langle N_j \rangle = \frac{1}{e^{(\epsilon_j - \mu)/T} - 1},$$

where $\mu \leq \epsilon_0$ is the chemical potential that indirectly fixes the average particle number

$$\langle N \rangle = \sum_j \langle N_j \rangle = \sum_j \frac{1}{e^{(\epsilon_j - \mu)/T} - 1}.$$

When Einstein read about this in a letter from Bose, he came up with some interesting consequences. For free particles in a three-dimensional box with volume $l^3$, the eigenfunctions are standing waves. In the thermodynamic limit $l \to \infty$, the energy levels are proportional to $p^2$ for $p \in \mathbb{R}^3$, the sum over energy levels can be approximated by an integral over $p$ and the numbers $\langle N_j \rangle$ turn into a function $\langle N(p) \rangle$. The statistics for bosons then say that for $\mu \leq 0$, the expected density of particles with momentum $p$ in the box is

$$\gamma(p) = \frac{\langle N(p) \rangle}{l^3} = \frac{1}{e^{(p^2 - \mu)/T} - 1}. \tag{2}$$

Since this increases with $\mu \leq 0$, this implies that the expected particle density, denoted by $\rho$, satisfies

$$\rho = \frac{1}{l^3} \int \langle N(p) \rangle dp \leq \int \frac{1}{e^{p^2/T} - 1} dp = c_0 T^{3/2} =: \rho_{\text{fc}} \tag{3}$$

for some constant $c_0$. We conclude that densities larger than $\rho_{\text{fc}}$ cannot be reached by defining a $\mu$ and following Bose statistics. But there is nothing stopping us from taking a box and adding particles until this density is exceeded! What happens when we do this is interpreted as *Bose–Einstein condensation (BEC)*: all particles in excess of $\rho_{\text{fc}}$ are assumed to be in the $p = 0$ (lowest energy) state so that they do not participate in the statistics; the lowest energy state is *macroscopically occupied.*[1][2]

[1] Note that this conclusion changes in one and two dimensions, where all $\rho \geq 0$ can be reached by choosing $\mu$ close enough to 0, and we do not have BEC at positive temperature.

[2] As in our simple example, this should be contrasted with the distribution for distinguishable particles. This is the *Maxwell–Boltzmann distribution*

$$\gamma(p) = \frac{\langle N(p) \rangle}{l^3} = \frac{1}{e^{(p^2 - \mu)/T}}. \tag{4}$$

This also has the property that particles concentrate in the lower lying levels, but nonetheless $\int \gamma \to \infty$ as $\mu \to 0$, so that we can reach all $\rho \geq 0$ by following these statistics and specifying a $\mu \leq 0$.

This analysis and the quantities $\gamma, \mu, \rho, \rho_{\text{fc}}$ will play a big role in this thesis. The 'fc' in $\rho_{\text{fc}}$ stands for 'free critical': it refers to the critical point of the non-interacting (free) Bose gas. For a fixed density $\rho$, the relation (3) can be inverted to a free critical temperature

$$T_{\text{fc}} = (\rho/c_0)^{2/3}, \tag{5}$$

below which we have BEC.

As mentioned before, BEC plays a role in both superfluidity and superconductivity, but the phenomenon has also been observed more directly. Gases of atoms can be trapped by magnetic fields and cooled to extremely low temperatures using lasers. In this setting, gases of rubidium and sodium atoms were observed to form a BEC in 1995 [10, 30], see Figure 2 for more information.

We should mention that the situation in this figure is more complicated than the case described by Bose and Einstein because of the presence of an external trap. An approximate description is given by the Gross–Pitaevskii equation [24, 46], which is accurate in a particular limit [36]. We will not consider external trapping potentials, but rather the *translation-invariant* or *homogeneous* case in which such a trap is absent.

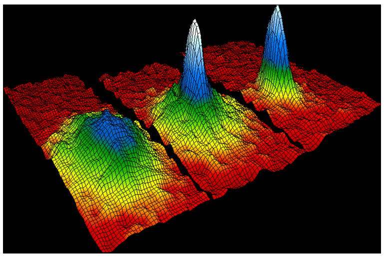

Figure 2: The momentum distribution of the particles in a gas of rubidium atoms as a function of $p_x$ and $p_z$. The plot on the left shows the distribution at approximately 200 nK. Although the density is highest for $p = 0$, there is no condensation. After lowering the temperature to approximately 100 nK (middle plot), a phase transition has taken place and a Bose–Einstein condensate has formed. Going to temperatures as low as 20 nK (right plot) causes the distribution to move closer to $p = 0$. Note that this is a system with an external trapping potential, which makes it different from the homogeneous (translation-invariant) set-up discussed in this thesis. This image came out of the experiments reported in [10]. Image credit: NIST/JILA/CU-Boulder.

As mentioned several times now, superfluidity and superconductivity are manifestations of Bose–Einstein condensation. It took particular effort to realize this for superconductivity as current in metals is transported by electrons, which are not bosons. In fact, they are particles that have the tendency to avoid each other, called fermions. As a consequence, condensation of electrons cannot occur, and it seems that BEC and superconductivity are unrelated. However, it it turns out that fermions can pair up in momentum space to form bosons, and these *can* form a condensate. This was first described by Bardeen, Cooper and Schrieffer in 1957 [6], but we will not discuss these ideas in this thesis.

Of more relevance to us here is the link between superfluidity and BEC. Since helium-4 particles are bosons, this connection is more evident and was already suggested by London [40] in 1937, but, ironically, it is less well understood today. We will say a little more about this later, but what is important now is that the main source of difficulty is the presence of strong interactions between the helium nuclei (see Figure 3), and that the description of BEC we just considered only applies to non-interacting particles.

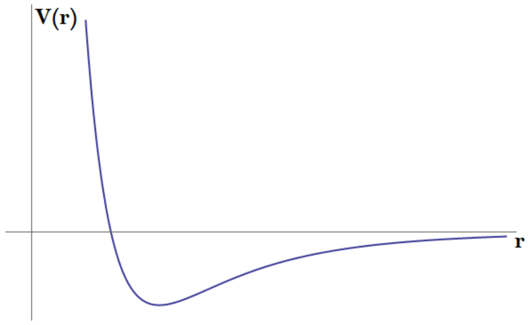


Figure 3: The potential between two helium nuclei $V$ as a function of the distance $r$. For short distances, it can be approximated by a hard-core potential (6), and it differs dramatically from the non-interacting case.

Feynman [16, 17] studied BEC in the presence of the interaction potential of Figure 3, and asked how the Bose–Einstein argument and the free critical temperature (5) are altered by it. His analysis is mostly qualitative and is based on a path integral description of the problem. Arguing that the potential resulted in an increased effective mass, Feynman predicted that the critical temperature would decrease compared to the free case, which had indeed been observed for liquid helium. He did not make any quantitative predictions.

To make such quantitative predictions, various simplifications were considered. The first one is to replace the interaction potential in the figure above with a hard-core potential with radius $a > 0$

$$V(x) = \begin{cases} \infty & |x| \leq a \\ 0 & |x| > a \end{cases}. \tag{6}$$

To simplify things further, it is common to study the so-called *dilute limit*. For a hard-core potential, the natural length scale is given by the radius $a$. We could compare this length scale to the one defined by the density: $\rho^{-1/3}$, the average distance between the particles. Diluteness now means that the particles meet only rarely, that is, the average distance between the particles is much bigger than the length scale of the potential, or

$$\rho^{1/3} a \ll 1. \tag{7}$$

This assumption is not valid for liquid helium, but it is for experiments with trapped atoms like the one in Figure 2. In any case, one can repeat Feynman's question: how is the free critical temperature (5) altered by the hard-core interaction?

Lee and Yang were the first to study this [33]. They used pseudopotential methods developed in [28, 32] to conclude that the shift in critical temperature should be proportional to $\rho^{1/3}a$. In the appendix of [33], they solve a simplified system, which gives

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + 1.79(\rho^{1/3}a) + o(\rho^{1/3}a)). \tag{8}$$

It is this kind of expression that we will be looking for in this thesis, but for a general class of potentials. To properly define the dilute limit (7) without reference to a hard-core potential, we consider a characteristic length scale of the potential that is known as the *scattering length* $a$. It coincides with the core radius for the hard-core potential. The mathematical definition is explained in [37].

Summarizing, the basic question that we try to answer in this thesis is:

**Question 1.1.** Can we prove a more accurate expression like (8) for general interactions in the dilute limit (7) from an approximate model for a weakly-interacting homogeneous Bose gas?

We will eventually discuss its affirmative answer. It is good to remember that this question came from studying BEC in superfluid helium, but that that particular problem remains intractable to this day. In its stead, the dilute setting has become a well-known and challenging object of study of its own. Indeed, the critical temperature (8) is higher than $T_{\mathrm{fc}}$, whereas the critical temperature of liquid helium is lower, which shows that the systems are quite different. Nonetheless, we have little hope of understanding the strongly-interacting case if we cannot even treat this weakly-interacting set-up, justifying the attention this problem has received (see [1] for an overview).

We have now reached the end of the non-technical part of the introduction. More details about the set-up and background of the problem will be given in the next section. The last section contains a more precise formulation of our goals, the approach and a summary of the results.

# 2 The weakly-interacting Bose gas and $T_{\mathrm{c}}$

## 2.1 Free energy and BEC

We start from the Hamiltonian for a gas of $N$ bosons that interact via a (periodized) repulsive pair potential $V^l$ in a three-dimensional box $[-l/2, l/2]^3$ with periodic boundary conditions:

$$H_N = \sum_{1 \leq i \leq N} -\Delta_i^l + \sum_{1 \leq i < j \leq N} V_{ij}^l.$$

Assuming the interaction only depends on the distance between the particles, this is translation-invariant, and we therefore write its second-quantized form in momentum space

$$H = \sum_p p^2 a_p^\dagger a_p + \frac{1}{2l^3} \sum_{p,q,k} \widehat{V}^l(k) a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p. \tag{9}$$

Here, only particular $p$ are included in the sum, as determined by the size of the box $l$.

So far we have not given a general definition of BEC. To do this, we need to say a little more about statistical mechanics, and address this in a rather mathematical setting. Since we are describing bosons, we are interested in the Hamiltonian (9) acting on the symmetric tensor product $\bigotimes_{\mathrm{SYM}}^N (L^2[-l/2, l/2]^3)$. A general state $\langle . \rangle_\omega$ is given by a density matrix $\omega$ on this Hilbert space. Its von Neumann entropy is

$$\langle S \rangle_\omega = \mathrm{Tr}[-\omega \ln \omega].$$

The canonical equilibrium, or Gibbs, state at temperature $T$ and particle density $\rho = N/l^3$ can be found be determining

$$\inf_{\omega \text{ on } \bigotimes_{\mathrm{SYM}}^N (L^2[-l/2,l/2]^3)} \langle H_N \rangle_\omega - T \langle S \rangle_\omega. \tag{10}$$

This is the *free energy* of the system at temperature $T$ and particle density $\rho$. We now say that a system displays BEC if the minimizer $\omega_{\rho,T}$ of (10) has an eigenvalue of order 1 [45]. Therefore, asking Question 1.1 for the full Hamiltonian (9) really means *finding minimizers to* (10)*, and studying the eigenvalues of their 1-particle reduced density matrices.* This is infeasible, so approximations will be needed.

As usual in statistical mechanics, it is easier to work in the grand canonical ensemble, in which the particle number is allowed to vary. The grand canonical Gibbs state at temperature $T$ and chemical potential $\mu$ is the minimizer of

$$\inf_{\omega \text{ on } \mathcal{F}^B(L^2[-l/2,l/2]^3)} \langle H \rangle_\omega - T \langle S \rangle_\omega - \mu \langle \mathcal{N} \rangle_\omega, \tag{11}$$

where $\mathcal{N}$ is the particle number operator $\mathcal{F}^B(L^2[-l/2, l/2]^3)$ is a bosonic Fock space (see [55] for a definition). The two quantities (10) and (11) are related by a Legendre transform as $l \to \infty$ (more on this *equivalence of ensembles* can be found in [47]).

In conclusion, the following question will be equally important to this thesis as Question (1.1):

**Question 2.1.** Can we find approximations to (10) and (11) in the dilute limit $\rho^{1/3} a \ll 1$?

To answer this question, one needs to find approximations to the spectrum of $H$, and we explain how this is usually done in the next subsection.

## 2.2 Bogoliubov's approach

We now discuss a crude version of the Bogoliubov approximation describing weakly-interacting Bose gases [9].

The first part of the Hamiltonian (9) is the kinetic energy and setting $V^l = 0$ gives the free case discussed before. The free Hamiltonian has the general form

$$\sum_p \epsilon(p) b_p^\dagger b_p, \tag{12}$$

with $\epsilon(p)$ a dispersion relation and $b_p^\dagger, b_p$ creation and annihilation operators.

Bogoliubov's strategy was to bring the Hamiltonian (9) into this form. As a first step, we could bring the number of $a$'s in (9) down to two. We use a so-called *c-number substitution*

$$a_0^\dagger, a_0 \longrightarrow \sqrt{N_0} = \left( N - \sum_{p \neq 0} a_p^\dagger a_p \right)^{1/2},$$

and, for simplicity, we also approximate the potential $V^l$ by a delta function (i.e. $\widehat{V}^l(k) \approx \widehat{V}^l(0)$ in (9)). The intuition behind the c-number substitution is BEC: a macroscopic ($O(N)$) occupation of the lowest energy state ($p = 0$). Of course, with this substitution there are still terms left with three or four $a_p^\dagger$ and $a_p$'s with $p \neq 0$, but these we throw out on the expectation that only $p = 0$ makes an $O(N)$ contribution, so that terms with one or zero $a_0^\dagger$ and $a_0$'s are of much lower order. We are left with the Hamiltonian

$$\sum_p p^2 a_p^\dagger a_p + \widehat{V}^l(0) \frac{N_0}{2l^3} \Big[ N_0 + \sum_{p \neq 0} 2 a_p^\dagger a_p + a_p^\dagger a_{-p}^\dagger + a_p a_{-p} \Big],$$

which can be made quadratic in the $a$'s by using $N_0 = N - \sum_{p \neq 0} a_p^\dagger a_p$ and throwing out any quartic terms. Now that we are left with something quadratic in creation and annihilation operators, we can bring it in the form (12) using a *Bogoliubov transformation.* Without going into the details, this involves defining new creation and annihilation operators as $b_p = c_1 a_p + c_2 a_p^\dagger$, where the constants $c_1$ and $c_2$ have to satisfy certain relations, see [55].

The resulting $\epsilon(p)$ in (12) is of the form

$$\epsilon(p) \sim \sqrt{p^2(p^2 + 2\widehat{V}(0)\rho)}. \tag{13}$$

This is known as the *Bogoliubov dispersion relation.* Landau [31] used this expression to provide a microscopic explanation for superfluidity. The linearity of the above expression for small $p$ is crucial, and it should be contrasted with a quadratic dependence on $p$ in absence of an interaction potential. We will not discuss this further.

A number of the steps in Bogoliubov's approach have been understood a lot better since 1947. The c-number substitution was justified in [38]. Careful analyses of the ground state energy and excitation spectrum include [12, 23, 35, 43, 49], and [50] contains a review. This thesis gives a different and, in our opinion, rather clear variational reformulation of Bogoliubov's approach, which emphasizes certain states rather than a truncation of the Hamiltonian. Our approach is also more complete in that fewer interaction effects are ignored. We will discuss it more in the next subsection, in the context of earlier work on Questions 1.1 and 2.1.

## 2.3 Previous results

To the best of our knowledge, the only rigorous result on the critical temperature for the full problem (11) is the upper bound established by Seiringer and Ueltschi using the Feynman–Kac formula [51]. It is not surprising that such results are thin on the ground: it remains impossible to prove BEC in the dilute limit at positive temperature, let alone determine at what temperature it occurs exactly. Results on the free energy of the full Hamiltonian can be found in [48, 58], and the ground state energy is discussed in [13, 15, 57, 39]. For the full model the phase transition to BEC is expected to be of second order.

As for approximate models, we already mentioned Lee and Yang's expression (8) [33] for the hard-core Bose gas. This expression can only be found in the appendix of their paper, perhaps because Lee and Yang considered their calculation to be physically inaccurate since it predicts a first—rather than the expected second—order phase transition. The fact that (8) was hidden in the appendix has presumably led to the widespread misconception that Lee and Yang only predicted a shift linear in $\rho^{1/3}a$, without saying anything about the sign or size of the constant [1, 7, 51, 52]. Even if Lee and Yang themselves did not really trust their result, it fits reasonably well with numerics: Monte Carlo methods [2, 29, 44] suggest that the form (8) is correct, but that the numerical value 1.79 should be closer to 1.3. It should be mentioned that this consensus emerged fairly recently; many different dependences on $\rho^{1/3}a$ have been suggested over the years [1], and even now conflicting results sometimes emerge [56].

So how do Lee and Yang approach this problem? They replace the boundary conditions resulting from the hard-core potential by a pseudopotential that should give the right wave function in the physically relevant region where all the particles are at least distance $2a$ from one another [28, 32]. They then assume that only s-wave scattering is important (i.e. the momentum of the particles is low), and show that replacing the potential by

$$8\pi a\delta(\boldsymbol{r})\partial_r r,$$

should yield the correct wave function. For smooth functions, this is simply a multiplication by a delta function, but the derivative does play a role for physical wave functions. All this leads to an excitation spectrum of Bogoliubov form, which can now be used to calculate the shift in the critical temperature (8).

Before we explain how this is done, let us point out that this claim in itself has led to some confusion. In a number of articles in which the weakly-interacting Bose is treated with field-theoretic methods—e.g. Bijlsma and Stoof [8] and Baym et al. [7], who find (8) with constants of 4.7 and 2.9, respectively—it is claimed that mean-field theories such as Bogoliubov's will simply give $T_c = T_{fc}$, or, in other words, no shift. One argument [1] goes as follows: a particle with momentum $p$ effectively has the energy

$$\epsilon(p) \sim \sqrt{p^2(p^2 + 2\widehat{V}(0)\rho)} = p^2\sqrt{1 + 2\widehat{V}(0)\rho/p^2} \approx p^2 + \widehat{V}(0)\rho,$$

in which the reader can recognize an approximation to Bogoliubov's dispersion relation. Inserting this constant shift of the energy levels into (2), we realize that now $\mu \leq \widehat{V}(0)\rho$. At this 'critical' $\mu$, the relation between $T$ and $\rho$ is still (3), and so the critical temperature does not change. However, one should be more careful in the use of (3) and the exact form of the dispersion relation.

In the Bogoliubov argument of the previous section, the occupation of the lowest energy state $N_0$ plays a crucial role. Dividing by the volume, we obtain a *condensate density* $\rho_0 = N_0/l^3$ that can now be regarded as a parameter. The dispersion relation Lee and Yang derive for the hard-core potential with radius $a$ is

$$\epsilon(p) \sim \sqrt{p^2(p^2 + 16\pi a\rho_0)}, \tag{14}$$

so, unlike (13), this gives a $\rho_0$-dependence. Furthermore, we should not define $\mu$ using (3), which just happened to be the minimizer of the free energy (11). Instead, for fixed $\rho$ and $\rho_0$, we should treat the remaining particles with density $\rho - \rho_0$ grand canonically, resulting in a grand canonical partition function that depends on $T$, $\rho$, $\rho_0$ and a chemical potential $\mu$. Recalling that there are only two independent parameters, one should now eliminate $\rho$ by calculating the value it takes at the minimum of the free energy for fixed $T$, $\rho_0$ and $\mu$, and then minimize over all $\rho_0$. The critical $\mu_c$ for fixed temperature is the one where the minimizing $\rho_0$ changes from $\rho_0 = 0$ (no BEC) to $\rho_0 > 0$ (BEC). Note that this definition is far more complicated than the naive conclusion $\mu_c = \widehat{V}(0)\rho$ above, but it is more correct. That was apparently clear to Lee and Yang, but it seems to have gone out of fashion, resulting in the false belief that the Bogoliubov spectrum cannot give a change in the critical temperature.

The treatment of the condensate $\rho_0$ as a separate parameter that defines the critical point is key to our analysis. Another important ingredient is a variational approach introduced by Critchley and Solomon [11]. They derive an upper bound to the free energy (11) by only considering a special class of density matrices in the minimization problem (11), namely *quasi-free states* (see e.g. [55]).[3]

[3] To put things into context; this approach has a fermionic counterpart, in which the trial states are quasi-free states on a fermionic Fock space (see [4] for details). This leads to the *BCS functional* [19, 25, 26] that serves as a model of superconductivity.

The upper bound resulting from quasi-free states is well-motivated. The first supporting argument is that Bogoliubov's approach reduces the Hamiltonian to an operator that is quadratic in the creation and annihilation operators, and that ground and Gibbs states of such operators are quasi-free states. A second is that quasi-free states have successfully served as trial states to establish correct bounds on the ground state energy of Bose gases [15, 22, 54], which is of course the $T = 0$ free energy.

Expressing $\langle H\rangle_\omega - T\langle S\rangle_\omega - \mu\langle \mathcal{N}\rangle_\omega$ for a general quasi-free state does lead to a complicated non-linear functional. Simplifying it somewhat by throwing out certain terms, Critchley and Solomon conclude that the model will reproduce Bogoliubov's conclusions.

In this thesis, we consider their functional without the simplifications, and use it as the approximate model in Questions 1.1 and 2.1. This is a variational reformulation of Bogoliubov's approach that is conceptually clear and more accurate. As indicated before, we use the condensate density $\rho_0$ to calculate a better approximation to the critical temperature in this variational setting.

# 3 The Bogoliubov free energy functional

## 3.1 Set-up and main questions

As explained, we are interested in considering the minimization problem (11) for quasi-free states. This leads to the functional that we study in this thesis. Properties of quasi-free states are listed in [55], but an important one is that they satisfy Wick's rule:

$$\begin{aligned}\langle a^\dagger_{p+k}a^\dagger_{q-k}a_q a_p\rangle_\omega = \langle a^\dagger_{p+k}a^\dagger_{q-k}\rangle_\omega\langle a_q a_p\rangle_\omega + \langle a^\dagger_{p+k}a_q\rangle_\omega\langle a^\dagger_{q-k}a_p\rangle_\omega \\ + \langle a^\dagger_{p+k}a_p\rangle_\omega\langle a^\dagger_{q-k}a_q\rangle_\omega.\end{aligned} \tag{15}$$

Applying the rule to the Hamiltonian (9) splits the expectation value of the difficult potential term into manageable bits: assuming translation invariance and $\langle a_p a_{-p}\rangle_\omega = \langle a^\dagger_{-p}a^\dagger_p\rangle_\omega$, the two (real-valued) functions $\gamma(p) := \langle a^\dagger_p a_p\rangle_\omega$ and $\alpha(p) := \langle a_p a_{-p}\rangle_\omega$ fully determine the energy expectation values.

In accordance with the rigorous justification of the c-number substitution [38], we put in a condensate by substituting $a_p \to a_p + \delta_{p,0}\sqrt{l^3}\sqrt{\rho_0}$ before we actually use Wick's rule. Mathematically, this is implemented by a Bogoliubov transformation (see [55]). To summarize, we now have three objects that define a state in our model.

- $\gamma$ describes the density of particles as a function of momentum $p$.
- $\rho_0 > 0$ indicates the presence of a Bose–Einstein condensate, whereas $\rho_0 = 0$ indicates that there is none.
- $\alpha \not\equiv 0$ shows off-diagonal long range order (ODLRO) and the presence of pairing in the system.

The triple $(\gamma, \alpha, \rho_0)$ has to lie in

$$\mathcal{D} = \{(\gamma,\alpha,\rho_0) | \gamma \in L^1((1+p^2)dp), \gamma(p) \geq 0, \alpha(p)^2 \leq \gamma(p)(1+\gamma(p)), \rho_0 \geq 0\}. \tag{16}$$

After the c-number substitution and the use of Wick's rule, we take the thermodynamic limit $l \to \infty$ to find the (grand canonical) *Bogoliubov free energy functional*[4]

$$\begin{aligned}\mathcal{F}_{\mu,T}(\gamma,\alpha,\rho_0) = &\int p^2\gamma(p)dp + \frac{1}{2}\widehat{V}(0)\rho^2 - \mu\rho - TS(\gamma,\alpha) \\ &+ \rho_0\int \widehat{V}(p)(\gamma(p)+\alpha(p))dp \\ &+ \frac{1}{2}\int \gamma(p)(\widehat{V}*\gamma)(p) + \alpha(p)(\widehat{V}*\alpha)(p)dp,\end{aligned} \tag{17}$$

with chemical potential $\mu \in \mathbb{R}$, density $\rho = \rho_0 + \rho_\gamma$, $\rho_\gamma = \int \gamma$, and an entropy defined in terms of $\beta(p) = \sqrt{(\gamma(p)+\frac{1}{2})^2 - \alpha(p)^2}$:

$$S(\gamma,\alpha) = \int \left(\beta(p)+\frac{1}{2}\right)\ln\left(\beta(p)+\frac{1}{2}\right) - \left(\beta(p)-\frac{1}{2}\right)\ln\left(\beta(p)-\frac{1}{2}\right)dp.$$

[4] This is up to factors of $2\pi$ that we decide to ignore here for brevity.

We will be thinking of the potential in this model as repulsive, $V \geq 0$, with positive Fourier transform, $\widehat{V} \geq 0$. Precise assumptions and a derivation of the functional can be found in Paper I.

The approximate free energy now is

$$F(T,\mu) = \inf_{(\gamma,\alpha,\rho_0)\in\mathcal{D}} \mathcal{F}(\gamma,\alpha,\rho_0). \tag{18}$$

The main questions addressed in this thesis are

**Questions 3.1.**

1. Given $\mu \in \mathbb{R}$ and $T \geq 0$, does the functional (17) have a minimizer in the domain (16)?
2. What does the $T/\mu$ phase diagram of the minimizers look like?
3. Which $\mu$'s and $T$'s correspond to the dilute limit $\rho^{1/3}a \ll 1$ and if a phase transition is present, can we expand $\mu_c$ in $\rho^{1/3}a$?
4. Can we expand the approximate free energy (18) in $\rho^{1/3}a$ in the dilute limit?

The first question is mostly of mathematical interest, but an affirmative answer is required to seriously consider the other problems. Together with the second question, it is discussed in Paper I. The remaining two questions are related to Questions 1.1 and 2.1. These are discussed in Paper II.

The reader may wonder about the following: a state with $\alpha = \langle a_p a_{-p}\rangle_\omega \neq 0$ does not have a fixed particle number. The problem therefore only has a natural formulation in terms of $\mu$ and $T$. Nonetheless, the definition of the dilute limit as $\rho^{1/3}a \ll 1$ suggests that we look at fixed $\rho$. We therefore consider a second variational problem involving $\mathcal{F}^{\mathrm{can}} = \mathcal{F} + \mu\rho$, or

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) = &\int p^2\gamma(p)dp + \frac{1}{2}\widehat{V}(0)\rho^2 - TS(\gamma,\alpha)\\ &+ \rho_0 \int \widehat{V}(p)(\gamma(p)+\alpha(p))dp\\ &+ \frac{1}{2}\int \gamma(p)(\widehat{V}*\gamma)(p) + \alpha(p)(\widehat{V}*\alpha)(p)dp,\end{aligned} \tag{19}$$

with $\rho_0 = \rho - \rho_\gamma$. The minimization problem only considers fixed $\rho$.

$$\begin{aligned}F^{\mathrm{can}}(T,\rho) &= \inf\{\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0=\rho-\rho_\gamma) \mid (\gamma,\alpha,\rho_0=\rho-\rho_\gamma)\in\mathcal{D}\}\\ &= \min\{f(\rho,\rho_0) \mid 0 \leq \rho_0 \leq \rho\},\end{aligned}$$

where

$$f(\rho,\rho_0) = \inf\{\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) \mid (\gamma,\alpha,\rho_0)\in\mathcal{D}, \rho_\gamma = \rho-\rho_0\}.$$

Note that $\rho$ is not the particle number in the states considered, but merely the average particle number. We will study both this minimization problem and (18), and switch between the two whenever convenient.

## 3.2 Tools and ideas

We now mention some key ideas that enter our analysis. A more complete summary of the ideas used in Paper II can be found in the Review.

**Paper I:**

- Since we are considering the dilute limit, or weak interactions, the physics is expected to be close to the non-interacting case. The functional describing the free gas is

$$\int p^2\gamma - TS(\gamma,0) - \mu\int\gamma. \tag{20}$$

Note that the minimizer of this functional for $\mu \leq 0$ is indeed (4).

- It can sometimes happen that no minimizer exists within a reasonable class of functions. We have already seen an example since
$$\int p^2\gamma - TS(\gamma, 0)$$
does not have a minimizer when we consider $\gamma \in L^1(1+p^2)$ with fixed $\rho > \rho_{\text{fc}}$. The reason is that any minimizing sequence will tend to a delta function at 0, which is no longer in the admissible set of $\gamma$'s. If we include a $\rho_0$ however, we end up with the same functional, but the remaining mass $\rho - \rho_{\text{fc}}$ can be put into the $\rho_0$. This means that a minimizer does exist within the set $\mathcal{D}$. Our model shows similar behaviour, and this will crucially enter in the proof of the existence of minimizers.

  Energetically, this comes down to
$$\mathcal{F}(\gamma + \rho_0\delta, \alpha + \rho_0\delta, 0) = \mathcal{F}(\gamma, \alpha, \rho_0) + \frac{1}{2}\widehat{V}(0)\rho_0^2,$$
so that adding mass to $\rho_0$ is even preferred over the formation of a delta function.

- Besides the above fact, the proof of existence of a minimizing triple $(\gamma, \alpha, \rho_0)$ of (18) for $T > 0$ and any $\mu$ uses standard techniques in the calculus of variations to extract a minimizer from a minimizing sequence. This has to be done in several steps and with various cut-offs to ensure that we can apply the standard theorems.

- The bounds used to prove the $T > 0$ existence deteriorate as $T \to 0$, and a separate argument in needed to show existence of a minimizing triple for $T = 0$. We are able to extract a minimizer from the $T > 0$ minimizers using the Arzelà–Ascoli theorem.

- The phase diagram follows from fairly simple arguments involving upper (in the form of trial states) and lower bounds on the free energy.

**Paper II:**

- As indicated before, the dilute limit $\rho^{1/3}a \ll 1$ suggests that we look at (19) with fixed $\rho$. However (even with a Lagrange multiplier), the presence of the convolution terms prevents us from using the Euler–Lagrange equations to find an explicit minimizer. The main idea therefore is to approximate
$$\inf_{\substack{(\gamma,\alpha,\rho_0)\\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\text{can}} \approx \inf_{\substack{(\gamma,\alpha,\rho_0)\\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\text{sim}} = \inf_{0\le\rho_0\le\rho}\left[\inf_{\substack{(\gamma,\alpha)\\ \rho_\gamma=\rho-\rho_0}} \mathcal{F}^{\text{sim}}\right]$$
where $\mathcal{F}^{\text{sim}}$ is a simplified functional that can be minimized explicitly. The Review outlines the other steps in this analysis.

## 3.3 Results and conclusions

Short answers to Questions 3.1, and also Questions 1.1 and 2.1 are listed below.

**Answers 3.2.** 1. Yes, minimizers exist. This, together with a similar theorem for the canonical case, is proven in Paper I.

2. The phase diagram is shown in Figure 4. It is derived in Paper I.

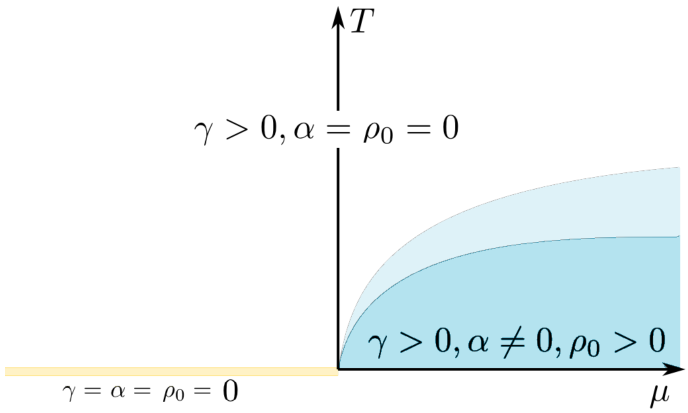


Figure 4: The grand canonical phase diagram of the model. No diluteness is assumed. At $\mu \le 0$ and $T = 0$, all quantities are zero, in particular there is no BEC. Increasing $T$ does not lead to a phase transition, although $\gamma$ becomes non-zero. For $\mu > 0$ fixed and $T = 0$, there is BEC. This remains the case when $T$ increases (darkest region), eventually leading to a phase transition somewhere in the lighter region before we enter the white region where $\rho_0 = 0$. We can only locate the phase transition precisely for $\mu \to 0$.

3. The dilute limit $\rho^{1/3}a \ll 1$ corresponds to $\mu \to 0$. In the limit $\widehat{V}(0) \to 8\pi a$, which is often considered, we find

$$\frac{\mu_{\mathrm{c}}}{8\pi} = 2\rho_{\mathrm{fc}}a - 0.226T^2a^2 + o(T^2a^2).$$

Canonically, we find a critical temperature

$$T_{\mathrm{c}} = T_{\mathrm{fc}}\left(1 + 1.49\rho^{1/3}a + o(\rho^{1/3}a)\right)$$

The constant 1.49 fits better with numerical results predicting 1.3 [2, 29, 44] than Lee and Yang's 1.79 from (8). Just like the latter, however, this model predicts a first-order phase transition, which is not expected to be correct. A more general statement can be found in Paper II.

4. Because of its variational formulation, this model gives upper bounds to the free energy of the full theory. These can indeed be expanded in $\rho^{1/3}a \ll 1$. This is explained in Paper II.

## 3.4 Outlook

We list open questions, starting from this model and gradually moving away from it.

1. This model gives an upper bound to the free energy, also at $T = 0$, which is the ground state energy. In the dilute limit, the exact ground state energy was predicted to be

$$4\pi a\rho^2 + \frac{512}{15}\sqrt{\pi}(\rho a)^{5/2} + o((\rho a)^{5/2})$$

by Lee, Huang and Yang [32]. Our model does reproduce the leading behaviour, but the second order only comes out correctly in the limit $\widehat{V}(0) \to 8\pi a$, which is not rigorous. A similar result was earlier obtained by Erdős, Schlein and Yau [15], but the exact upper bound has in fact been shown by Yau and Yin [57]. One could ask whether this model can be improved so that it does reproduce the correct $T = 0$ upper bound without the limit $\widehat{V}(0) \to 8\pi a$. Such a model would then presumably also give more accurate free energy expansions for $T > 0$.

2. The results summarized above are similar in one and two dimensions. This is unexpected, since the Mermin–Wagner–Hohenberg theorem [27, 42] says there cannot be BEC in one and two dimensions at positive temperature. This shows that the minimizer in the class of quasi-free states does not always have the right physical properties, even when its energy is very close to the real minimum. It would be interesting to see if the class of trial functions can be extended to better reflect the physical properties of the system, although it is difficult to see what can be done without Wick's rule, which has to be given up if one wants to go beyond quasi-free states.

   In two dimensions, moreover, there is the possibility of a Kosterlitz-Thouless transition, so one could calculate the critical temperature predicted by this model and investigate whether there is a relation with the phase transition predicted here.

3. Another false prediction of the model is that the phase transition is of first order, a property that is likely to be shared with any analysis based on Bogoliubov's original approach. It is unclear how to adapt the model so that it gives the second-order phase transition that is predicted for the full Hamiltonian.

4. Dynamics do not play any role in this thesis, but they have recently been considered in a variational setting in [3], where the authors restrict the time evolution of a Bose gas to quasi-free states.

5. This model describes a homogeneous (translation-invariant) system, but experiments with dilute cold atomic gases often involve a (harmonic) trap. One could ask whether that set-up can also be described with a variational model.

6. The previous point is related to the question whether the predicted shift in critical temperature due to interactions can actually be measured. For harmonic traps, a linear shift in the critical temperature has indeed been measured [14, 21, 53], but it cannot be compared with the predictions discussed in this thesis because the effect of the trap, expected to lower rather than raise the critical temperature, is simply too big. Recently, a BEC was also created in a uniform potential [20]. The measurements are not precise enough, however, to measure the critical temperature shift directly, but even if they were, in this set-up the finite size effects due to the boundedness of the trap are expected to be six times larger than the shift caused by the interaction. In the words of [52], 'we are thus still lacking a direct measurement of the historically most debated [$T_c$] shift'.

7. On a different note, it seems that the trapped set-up is often related to the homogeneous case using a *local density approximation* [52]. It assumes that the gas is locally described by the translationally-invariant theory with a chemical potential $\mu(x) = \mu - V^{\text{trap}}(x)$. Given the confusion surrounding $\mu$ discussed in (2.3), it seems that a better theoretical understanding of this approximation and the role of $\mu$ is called for.

8. As indicated, the theoretical challenges surrounding BEC are considerable. Mathematically, its existence at positive temperature has never been shown in a continuous system, and a calculation of the critical temperature in the dilute limit is therefore completely out of reach.

9. As shown in Paper I, this model has the property that $\alpha \not\equiv 0$ if and only if $\rho_0 > 0$. That is to say, ODLRO and BEC go together. Both have a connection with superfluidity [5, 34] that is not entirely understood. This thesis does not shed any light on that of course, as we have avoided a discussion of the relation between $\alpha$ and superfluidity altogether.

10. The original motivation for the questions discussed in this thesis came from liquid helium, but since that is a strongly-interacting system, no relevant conclusions can be drawn from this analysis. A set-up with strong interactions that has recently been studied is the *unitary Bose gas* [18, 41], in which the scattering length tends to infinity. In a way, it is the opposite of the dilute gas studied here.

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# Review

## Calculation of the Critical Temperature of a Dilute Bose Gas in the Bogoliubov Approximation

# Calculation of the Critical Temperature of a Dilute Bose Gas in the Bogoliubov Approximation

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We give a natural variational reformulation of the famous Bogoliubov approximation for a weakly-interacting translation-invariant Bose gas. The resulting variational model turns out to be a more accurate approximation than the usual Bogoliubov approach. It allows us, moreover, to give a novel derivation of the change of the critical temperature in the dilute limit. This problem has been extensively studied going back to a fundamental paper of Lee and Yang. Our expression for the critical temperature differs from that of Lee and Yang and subsequent theoretical results and is, indeed, in better agreement with numerical simulations. We also review general properties of the Bogoliubov variational model.

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*Introduction.* Despite experimental realizations of Bose–Einstein condensation (BEC) in interacting cold atomic gases in 1995, and in a variety of systems since, it remains an open problem to theoretically demonstrate its occurrence in translation-invariant systems [19, 25], let alone derive the critical temperature.

For a *non-interacting*, or *free*, Bose gas with density $\rho$, the textbook argument by Einstein shows that the critical temperature (in units $\hbar = 2m = k_B = 1$) is

$$T_{\mathrm{fc}} = 4\pi\zeta(3/2)^{-2/3}\rho^{2/3}. \tag{1}$$

So how does an interaction change this *free critical temperature*? Feynman [9] used path integrals to qualitatively answer this question for liquid helium. He predicted that the potential results in an increased effective mass, which lowers the critical temperature – something that had already been measured.

To make quantitative predictions, various simplifications were considered. For a hard-core Bose gas with core radius (or scattering length) $a$, one can *assume that the gas is dilute* and apply perturbation theory. The relevant parameter is $\rho^{1/3}a \ll 1$, which says that the particles tend to be far apart on the scale of the interaction.

Studying this set-up, Lee and Yang [17] replace the hard-core potential with a pseudopotential [14, 16] and simplify the resulting Hamiltonian with the Bogoliubov approximation [5]. They conclude that the shift in the critical temperature should be proportional to $\rho^{1/3}a$

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + 1.79(\rho^{1/3}a) + o(\rho^{1/3}a)), \tag{2}$$

see the appendix of [17].

Here, we improve on this in two ways. Much progress has been made on the theoretical analysis of Bose gases over the last few years [19, 25], so that we can treat a general class of potentials without reverting to pseudopotentials. For this class of potentials, we derive a more accurate version of (2) (where $a$ is now the *scattering length*) since, although Bogoliubov's approximation cannot give the right energy to second order in $\rho^{1/3}a$, it was recently realized [7] that it gives the correct first-order term if the approximation is done carefully [31].

Indeed, our main result is a calculation of an expression like (2) for a general class of potentials that also agrees better with numerics.

*Background.* Expressions for $T_{\mathrm{c}}$ of the dilute Bose gas have been derived in many different models. We should, after all, first try to understand dilute systems before we can have any hope of understanding condensation in strongly interacting systems such as liquid helium.

Keeping this in mind, the reader may have noticed the discrepancy between the observed decrease in $T_{\mathrm{c}}$ for helium and (2). Indeed, some early theoretical results such as [8] disagree with the predicted temperature increase in (2). There was also a lot of debate on whether the linear dependence on $\rho^{1/3}a$ is correct ([11–13] predict exponents of 1/2, 3/2 and 1/2, respectively). Nonetheless, up to the precise value of the constant 1.79, (2) is still expected to hold true. That it does not apply to helium does not have to be too surprising: liquid helium is not weakly interacting.

The critical temperature cannot be determined without approximations, although [27] contains an exact upper bound. It is far from the desired form (2) in that the power of the correction is $(\rho^{1/3}a)^{1/2}$.

The constant 1.79 in (2) has been recalculated with field theoretic methods (see Andersen's review [1]). In particular, Bijlsma and Stoof [4] and Baym et al. [3] find (2) with constants of 4.7 and 2.9, respectively.

Numerical studies with Monte Carlo methods now seem to agree that the value should lie around 1.3 [2, 15, 23]. We find a constant of 1.49.

*Set-up.* We start from the Hamiltonian for a gas of $N$ bosons with a repulsive pair interaction $V$ in a three-dimensional box $[-l/2, l/2]^3$ and periodic boundary conditions. In units $\hbar = 2m = k_B = 1$,

$$H_N = \sum_{1\leq i\leq N} -\Delta_i + \sum_{1\leq i<j\leq N} V_{ij}. \tag{3}$$

The *canonical* equilibrium, or Gibbs, state at temperature $T$ and particle density $\rho = N/l^3$ can be found by minimizing

$$\inf_{\omega} \langle H_N - TS\rangle_\omega, \tag{4}$$

where $\omega$ is an $N$-boson state.

As usual, it is easier to work in the grand canonical ensemble. We consider a Hamiltonian $H$ that acts as $H_N$ on the $N$-particle sector of the bosonic Fock space. The *grand canonical* Gibbs state at temperature $T$ and chemical potential $\mu$ is the minimizer of

$$\inf_{\omega} \langle H - TS - \mu\mathcal{N}\rangle_\omega, \tag{5}$$

where $\omega$ is now a state on the bosonic Fock space, $\mathcal{N}$ is the particle number operator and the infimum itself is the *free energy.*

Throughout this paper we will be working in the *thermodynamic limit* $l \to \infty$. The two quantities (4) and (5) are then related by a Legendre transform.

We now say that a system displays *BEC* if the 1-particle reduced density matrix of the minimizing $\omega$ of (5) has an eigenvalue of order 1 [24]. Therefore, *one really needs to find minimizers to* (5) *to determine* $T_c$.

This cannot be done exactly. The exact free energy (5) has only been analysed in [26, 29]; all other results in the literature, such as [30], concern approximations. We will study one such model, first introduced in [6]. It restricts the minimization problem (5) to *quasi-free states*, resulting in a variational upper bound on the free energy.

There are good arguments why this upper bound is accurate. The first is that Bogoliubov's approach renders the Hamiltonian quadratic in creation and annihilation operators. Ground and Gibbs states of such Hamiltonians are quasi-free states; exactly the states considered in our minimization problem. Also, quasi-free states have already proven to be good trial states for the ground state energy of Bose gases [7, 10, 28], and may therefore also be for the free energy.

Can we use this upper bound to approximate $T_c$? As we will soon see, expressing $\langle H - TS - \mu\mathcal{N}\rangle_\omega$ for a general quasi-free state leads to a non-linear functional (8). Linearizing the functional by removing the terms quartic in creation and annihilation operators, the authors of [6] conclude that the Gibbs state coincides with that of Bogoliubov's (approximated) Hamiltonian.

In this paper, we consider the functional *without* the linearization, motivated by the discovery in [7] that the correct first-order energy is only found when the terms quartic in creation and annihilation operators are included. This gives a variational calculation of $T_c$ that is also more accurate.

*Model.* We consider the Hamiltonian (3), make the assumption that we are in the *translation-invariant* case, and write its second-quantized form in momentum space

$$H = \sum_p p^2 a_p^\dagger a_p + \frac{1}{2l^3}\sum_{p,q,k} \widehat{V}(k) a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p. \tag{6}$$

We expect some particles to form a condensate at zero momentum. We therefore mimic Bogoliubov's c-number substitution (justified in [20]) by using a Bogoliubov transformation to implement a *condensate density* $\rho_0 \geq 0$, effectively replacing $a_0 \to a_0 + \sqrt{l^3\rho_0}$. A minimizer with $\rho_0 > 0$ will *indicate the presence of BEC*, whereas $\rho_0 = 0$ signifies its absence.

We evaluate the expectation value of the resulting Hamiltonian for quasi-free states only, so that we can use Wick's rule to split $\langle a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p\rangle$ as

$$\langle a_{p+k}^\dagger a_{q-k}^\dagger\rangle\langle a_q a_p\rangle + \langle a_{p+k}^\dagger a_q\rangle\langle a_{q-k}^\dagger a_p\rangle + \langle a_{p+k}^\dagger a_p\rangle\langle a_{q-k}^\dagger a_q\rangle. \tag{7}$$

Assuming translation invariance and $\langle a_p a_{-p}\rangle = \langle a_{-p}^\dagger a_p^\dagger\rangle$, the two (real-valued) functions $\gamma(p) := \langle a_p^\dagger a_p\rangle \geq 0$ and $\alpha(p) := \langle a_p a_{-p}\rangle$, together with the number $\rho_0$, fully determine the expectation value in (5).

Here, $\gamma(p)$ is the *density of particles with momentum* $p$, and $\alpha$ describes *the presence of pairing in the system.* We have off-diagonal long range order (ODLRO) if $\alpha$ is not the zero-function, which is related to superfluidity [18]. It is well-known that the two functions have to satisfy $\alpha^2 \leq \gamma(\gamma + 1)$.

Taking the thermodynamic limit $l \to \infty$, we have now evaluated the expectation in (5) over *Bogoliubov trial states*: quasi-free states with an added condensate.

The *Bogoliubov free energy functional* is then

$$\begin{aligned}\mathcal{F}_{\mu,T}(\gamma,\alpha,\rho_0) &= (2\pi)^{-3}\int p^2\gamma(p)dp - \mu\rho - TS(\gamma,\alpha)\\ &+ \rho_0(2\pi)^{-3}\int \widehat{V}(p)(\gamma(p)+\alpha(p))dp + \frac{1}{2}\widehat{V}(0)\rho^2\\ &+ \frac{1}{2}(2\pi)^{-6}\int \gamma(p)(\widehat{V}*\gamma)(p) + \alpha(p)(\widehat{V}*\alpha)(p)dp,\end{aligned} \tag{8}$$

with chemical potential $\mu \in \mathbb{R}$, density $\rho = \rho_0 + \rho_\gamma$ (i.e. a sum of the condensate density $\rho_0$ and the density of particles with positive momentum $\rho_\gamma = (2\pi)^{-3}\int \gamma$). The entropy, defined in terms of $\beta(p) = \sqrt{(\gamma(p)+\frac{1}{2})^2 - \alpha(p)^2}$, is

$$S(\gamma,\alpha) = (2\pi)^{-3} \int \left(\beta(p) + \frac{1}{2}\right) \ln\left(\beta(p) + \frac{1}{2}\right) - \left(\beta(p) - \frac{1}{2}\right) \ln\left(\beta(p) - \frac{1}{2}\right) dp. \tag{9}$$

A precise derivation, including a calculation of the entropy for quasi-free states, can be found in the appendix of [21].

For a canonical formulation with fixed *average* density $\rho$ and temperature $T$, we consider

$$\mathcal{F}^{\mathrm{can}}_{\rho,T} = \mathcal{F}_{\mu,T}(\gamma,\alpha,\rho_0) + \mu\rho, \tag{10}$$

and only states with $\rho_0 + \rho_\gamma = \rho$. This amounts to evaluating the expectation in (4) for Bogoliubov states.

In what follows, we often drop the subscripts of $\mathcal{F}^{\mathrm{can}}_{\rho,T}$ and $\mathcal{F}_{\mu,T}$. Note that, in contrast to (4) and (5), the infima of these functionals are not automatically related by a Legendre transform because of the restricted minimization. We will see that the canonical infimum is not convex, and that the relation only goes one way (34).

*Results.* We assume that the two-body interaction potential is repulsive, integrable and bounded. Its Fourier transform is assumed to be positive and has its maximum at zero since $V \geq 0$.

The gas is dilute, $\rho^{1/3}a \ll 1$, and the temperature is approximately $T_{\mathrm{fc}}$. Note that this implies that $\sqrt{T}a \ll 1$, a limit that we make extensive use of. We also use the first-order Born approximation of the scattering length $a$, i.e. $\widehat{V}(0) = \int V \approx 8\pi a$, and the fact that we can expand

$$\widehat{V}(p) = \widehat{V}(0) + Ca^3p^2 + o(a^3p^2), \tag{11}$$

where the first derivative is absent since $\widehat{V}$ has its maximum at zero, and the second derivative is assumed to be of order $a^3$ (in accordance with its units).

The following results are proved in our earlier paper [21]. They provide some necessary background.

**THEOREM 1.** *There exist minimizers for both the grand canonical* (5) *and canonical minimization problem* (4) *when the minimization is restricted to Bogoliubov trial states only (resulting in a minimization of the functionals* (8) *and* (10)*, respectively).*

For these minimizers, we investigate whether a phase transition occurs.

**THEOREM 2.** *The grand canonical phase diagram of the model is shown in FIG. 1. In particular, there is a phase transition at positive $T$ for all fixed $\mu > 0$. Also, $\alpha \neq 0$ iff $\rho_0 > 0$, so that BEC and ODLRO always occur together in this model.*

*Canonically, there is a phase transition at positive $T$ for all fixed $\rho > 0$.*

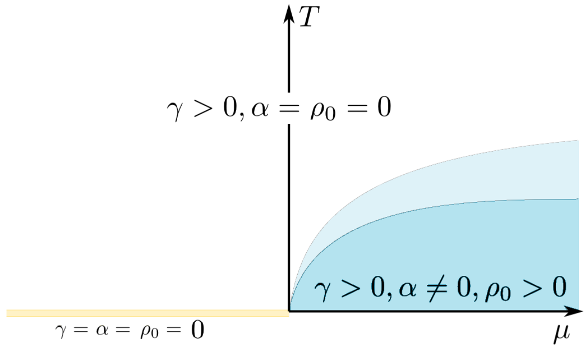


FIG. 1: The grand canonical phase diagram of the model. No diluteness is assumed. At $\mu \leq 0$ and $T = 0$, all quantities are zero, in particular there is no BEC. Increasing $T$ does not lead to a phase transition, although $\gamma$ becomes non-zero. For $\mu > 0$ fixed and $T = 0$, there is BEC. This remains the case when $T$ increases (darkest region), eventually leading to a phase transition somewhere in the lighter region before we enter the white region where $\rho_0 = 0$. We can only locate the phase transition exactly for $\mu \to 0$; a further analysis shows that this corresponds to the dilute limit studied in THEOREM 3.

We now turn to the main result: the calculation of the critical temperature. The definition of diluteness $\rho^{1/3}a \ll 1$ suggests that we look at the canonical functional (10) first, but we also consider the grand canonical case.

**THEOREM 3.** *Consider the canonical problem* (4) *restricted to Bogoliubov trial states with $\rho = \rho_0 + \rho_\gamma$ fixed, resulting in the canonical functional* (10)*. The critical temperature, defined by the properties $\rho_0 > 0$ if $T > T_{\mathrm{c}}$, $\rho_0 = 0$ if $0 \leq T < T_{\mathrm{c}}$, is*

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + \kappa(\rho^{1/3}a) + o(\rho^{1/3}a)), \tag{12}$$

*where $\kappa = 1.49$ in the limit $\widehat{V}(0) \to 8\pi a$.*

*The phase transition can also be identified in the grand canonical model* (5)*, i.e. for minimizers of* (8) *with fixed $T$ and $\mu$. It is a first-order phase transition.*

Note that the constant 1.49 is in reasonable agreement with the numerical consensus of 1.3 [2, 15, 23]. The proof relies on a careful expansion of the free energy.

*Proof of THEOREM 3.* We fix $T$ and set out to find the critical density $\rho_{\mathrm{c}}$, which can easily be inverted to (12).

*Outline.* We could try to minimize the functional by solving the Euler–Lagrange equations of (8). However, the terms with convolutions give non-local contributions of $\widehat{V} * \gamma$ and $\widehat{V} * \alpha$. Even with a Fourier transform, this cannot be solved.

We therefore approximate these terms so that we obtain a functional $\mathcal{F}^{\mathrm{sim}}$ that *can* be minimized explicitly in $\gamma$ and $\alpha$. We expand the resulting energy integrals, and finally minimize in $\rho_0$ to determine whether it is zero or not.

To sketch this once more,

$$\inf_{\substack{(\gamma,\alpha,\rho_0)\\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\mathrm{can}} \approx \inf_{0\le\rho_0\le\rho} \inf_{\substack{(\gamma,\alpha)\\ \rho_\gamma=\rho-\rho_0}} \mathcal{F}^{\mathrm{sim}}, \tag{13}$$

where the infimum over $\gamma$ and $\alpha$ is calculated explicitly, then expanded in $\sqrt{T}a \ll 1$, and finally minimized in $\rho_0$.

*Step 1a.* To approximate the convolution term involving $\gamma$, we use a comparison with the free Bose gas. Its energy is given exactly by the functional

$$\mathcal{F}_0(\gamma) = (2\pi)^{-3}\int p^2\gamma(p)dp - TS(\gamma,0), \tag{14}$$

whose minimizer for fixed $\rho$ is

$$\gamma_{\mu(\rho)}(p) = \frac{1}{e^{(p^2-\mu(\rho))/T}-1}, \tag{15}$$

where $\mu(\rho) \le 0$ is such that $(2\pi)^{-3}\int \gamma_{\mu(\rho)} = \rho$. This definition only works for $\rho \le \rho_{\mathrm{fc}}$, where the *free critical density* $\rho_{\mathrm{fc}}$ is characterized by $\mu(\rho_{\mathrm{fc}}) = 0$ (leading to the inverted expression of (1)). We define $\mu(\rho) = 0$ for $\rho \ge \rho_{\mathrm{fc}}$.

We would like to show that the minimizing $\gamma$ for the interacting problem lives on the same scale as $\gamma_0$, that is, most of the particles have momentum $|p| \le O(\sqrt{T})$. Indeed, a careful comparison shows that the minimizer has to satisfy

$$\mathcal{F}_0(\gamma_{\mu(\rho_\gamma)}) \le \mathcal{F}_0(\gamma) \le \mathcal{F}_0(\gamma_{\mu(\rho)}) + \rho^2\widehat{V}(0), \tag{16}$$

which says that the energy does not deviate much from the minimal energy in the free case. Because of the $\int p^2\gamma$ term, this means that $\gamma$ cannot be very large for $|p| \gg \sqrt{T}$ (see [22] for a precise statement).

For $|p| \le O(\sqrt{T})$, (11) implies

$$|\widehat{V}(p) - \widehat{V}(0)| = O(a(\sqrt{T}a)^2) \ll a. \tag{17}$$

Since $\gamma$ is only large on $|p| \le O(\sqrt{T})$, we can approximate $(2\pi)^{-3}\widehat{V} * \gamma \approx \widehat{V}(0)\rho_\gamma$.

To be more precise: a careful analysis in [22] shows

$$\left|(2\pi)^{-3}\int \widehat{V}(p)\gamma(p)dp - \widehat{V}(0)\rho_\gamma\right| = O(T^{3/2}a(\sqrt{T}a)^{3/2}), \tag{18}$$

and similar estimates for the term involving the convolution. These estimates can be further refined by narrowing the energy difference in (16).

*Step 1b.* The strategy for the convolution term with $\alpha$ is different. Following ideas in [7], we expect $\alpha$ to be related to the scattering solution $w$. It is defined by

$$-\Delta w + \frac{1}{2}Vw = 0, \tag{19}$$

with $w(x) \to 1$ as $|x| \to \infty$.

To work towards a good approximation for $\alpha$, we define

$$\alpha_0 := (2\pi)^3 t_0\delta_0 - \frac{\rho_0 + t_0}{2}\frac{\widehat{Vw}(p)}{p^2}, \tag{20}$$

where $-\rho_0 \le t_0 \le 0$ is an additional parameter that will be tuned to achieve a self-consistency equation $\int(\alpha - \alpha_0) = 0$. Note that $\alpha$ itself will in general not be integrable.

The motivation for defining $\alpha_0$ in this way is as follows: at momentum scales bigger than $Ta$, we expect $\alpha$ to resemble the second contribution above. Its structure on smaller scales is more complicated, but the exact shape is irrelevant. We approximate this part by a $\delta$-function. We will eventually optimize our approximation by determining $t_0$ so that $\int(\alpha - \alpha_0) = 0$.

How does the guess (20) help us? We add and subtract terms to replace the convolution term with $\alpha$ by

$$\int (\alpha - \alpha_0)(p)(\widehat{V} * (\alpha - \alpha_0))(p)dp, \tag{21}$$

which we later show to be small for the minimizing $\alpha$. Of course, by doing this we have introduced terms involving $\widehat{V} * \alpha_0$, which may seem like a problem. However,

$$(2\pi)^{-3}\widehat{V} * \alpha_0(p) = (\rho_0 + t_0)\widehat{Vw}(p) - \rho_0\widehat{V}(p), \tag{22}$$

so that no convolution terms remain in our functional. This has the added effect that $\widehat{V}$ gets replaced by $\widehat{Vw}$ in the term linear in $\alpha$, but this Fourier transform is well-defined and satisfies $\widehat{Vw}(0) = 8\pi a$. For simplicity of the resulting functional, we make sure to obtain a similar replacement for the $\rho_0\int\widehat{V}\gamma$-term.

*Step 1c.* To specify (13) and make use of the previous two steps, we prove upper and lower bounds. The errors in our approximation are

$$\begin{aligned}
E_1 &:= \frac{1}{2}(2\pi)^{-6}\int (\alpha - \alpha_0)(p)(\widehat{V} * (\alpha - \alpha_0))(p)dp\\
E_2 &:= \left|\rho_0(2\pi)^{-3}\int \gamma(p)\widehat{V}(p)dp - \widehat{V}(0)\rho_0\rho_\gamma\right|\\
E_3 &:= \left|\rho_0(2\pi)^{-3}\int \gamma(p)\widehat{Vw}(p)dp - \widehat{Vw}(0)\rho_0\rho_\gamma\right|\\
E_4 &:= \Big|\frac{1}{2}(2\pi)^{-6}\int \gamma(p)(\widehat{V} * \gamma)(p)dp\\
&\qquad - \frac{1}{2}\widehat{V}(0)\rho_\gamma^2 - \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4\Big|.
\end{aligned} \tag{23}$$

Following Steps 1a and 1b, the reader can now derive a simplified functional $\mathcal{F}^{\mathrm{sim}}$ satisfying

$$\begin{aligned}
-E_2 - E_3 - E_4 \le \mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,\rho_0)\\
\le E_1 + E_2 + E_3 + E_4.
\end{aligned} \tag{24}$$

The full expression for $\mathcal{F}^{\mathrm{sim}}$ is given in [22]. We will use (24) to prove that $\mathcal{F}^{\mathrm{sim}}$ really is a good approximation to the energy in Step 2c.

*Step 2a.* Now that we have $\mathcal{F}^{\text{sim}}$, we will calculate and expand its minimal energy as a function of $\rho$ and $\rho_0$. It turns out that we need to expand to order $T^4a^3 = T^{5/2}(\sqrt{T}a)^3$ to derive (12).

The part of $\mathcal{F}^{\text{sim}}$ that depends on $\gamma$ and $\alpha$ is

$$(2\pi)^{-3}\Big[\int p^2\gamma(p)dp + \frac{1}{4}\rho_0^2\int\frac{\widehat{Vw}(p)^2}{p^2}dp + \rho_0\int\widehat{Vw}(p)(\gamma(p)+\alpha(p))dp\Big] - TS(\gamma,\alpha). \tag{25}$$

Given $\rho_0$, this has minimizers $\gamma^{\rho_0,\rho}$ and $\alpha^{\rho_0,\rho}$. The dominant contribution of (25) to the energy $\mathcal{F}^{\text{sim}}(\gamma^{\rho_0,\rho},\alpha^{\rho_0,\rho},\rho_0)$ is

$$(2\pi)^{-3}T\int\ln\big(1-e^{-T^{-1}\sqrt{(p^2+\delta)^2+2(p^2+\delta)(\rho_0+t_0)\widehat{Vw}(p)}}\big)dp, \tag{26}$$

which resembles the energy of the free gas.

*Step 2b.* We now expand (26). To do this, we judiciously define

$$\rho_0 = \frac{\sigma}{8\pi}T^2a,\quad \rho = \rho_{\text{fc}} + \frac{k}{8\pi}T^2a,\quad \delta = dT^2a^2,\quad t_0 = \frac{\tau}{\sigma}\rho_0 \tag{27}$$

where $\sigma, k, \delta, \tau$ are parameters of order 1.

Changing variables $p \to Tap$ and using (11), we expand (26) for $\sqrt{T}a \ll 1$. In the limit $\widehat{V}(0) \to 8\pi a$, this gives

$$T^{5/2}f_0 + T^2a^2\rho_{\text{fc}}(d+(1+\theta)\sigma) - \frac{1}{12\pi}T^4a^3\left((d+2(1+\theta)\sigma)^{3/2}+d^{3/2}\right) + o(T^4a^3), \tag{28}$$

where $T^{5/2}f_0 = \mathcal{F}_0(\gamma_{\mu(0)})$ is the free gas energy. To simplify the expressions, we assume $\widehat{V}(0) \to 8\pi a$ from now on; what remains of the calculation can be done in the same way for other values of $\widehat{V}(0)$.

Of course, there is a relation between $d$, $k$ and $\sigma$, since $d$ was a Lagrange multiplier. We eliminate $d$ by calculating, expanding and solving $\int\gamma^{\rho_0,\rho} = \rho - \rho_0$, finding

$$d = \left(\frac{(\sigma-k)^2 - 2(\sigma+\tau)}{2(\sigma-k)}\right)^2. \tag{29}$$

*Step 2c.* We now use (24) to show that we can accurately approximate the energy. We claim the minimizers have to satisfy

$$|\mathcal{F}^{\text{can}}(\gamma,\alpha,\rho_0) - \mathcal{F}^{\text{sim}}(\gamma^{\rho_0,\rho},\alpha^{\rho_0,\rho},\rho_0) + \zeta T^4a^3| = o(T^4a^3), \tag{30}$$

where $\zeta T^4a^3$ is used to denote the constant in $E_4$ (23). There are two bounds to show.

The first follows from the lower bound in (24), and the a priori results from Step 1a. Note that no a priori information on $\alpha$ and $E_1$ is needed.

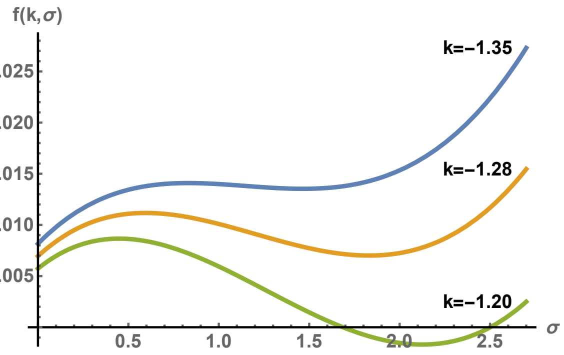


FIG. 2: Plots of the part of the free energy $f(k,\sigma)$ that depends on $k$ and $\sigma$ (i.e. between the square brackets in the second line of (33)) for three values of $k$. For $k = -1.35$, $\sigma = \rho_0 = 0$ gives the lowest energy: no BEC. For $k = -1.20$, the minimum occurs at some $\rho_0 > 0$: BEC. The critical value is $k_c = -1.28$.

The second uses the upper bound in (24). We simply verify that all errors in (23) are $o(T^4a^3)$ for $\gamma^{\rho_0,\rho}$ and $\alpha^{\rho_0,\rho}$. This is only non-trivial for $E_1$, for which it suffices to choose $\tau$ such that $\int(\alpha^{\rho_0,\rho} - \alpha_0) = 0$. We conclude

$$\tau = -\frac{2(\sigma+\tau)}{\sqrt{d+2(\sigma+\tau)}+\sqrt{d}} + o(1), \tag{31}$$

which can be used to eliminate $\tau$.

*Step 3.* We have now reduced (13) to

$$\inf_{\substack{(\gamma,\alpha,\rho_0)\\ \rho_0+\rho_\gamma=\rho}} \mathcal{F}^{\text{can}} = \inf_{\sigma\geq 0} f(k,\sigma) + o(T^4a^3), \tag{32}$$

where

$$f(k,\sigma) = T^{5/2}f_0 + \widehat{V}(0)\rho^2 + \zeta T^4a^3 + T^4a^3\left[\frac{1}{8\pi}\left(\frac{(\sigma-k)^3}{12} - \sigma^2\Big(\frac{1}{2}+\frac{1}{2+\sigma-k}\Big)\right)\right]. \tag{33}$$

We can determine $\rho_c$ by fixing $k$ and checking when the minimizing $\sigma$ changes from zero to non-zero, as illustrated in FIG. 2. We find $\rho_c = \rho_{\text{fc}} - 1.28T^2a/8\pi$, which can be rewritten as the desired $T_c$ (12).

*Step 4.* We are left with the grand canonical formulation and the order of the phase transition. By (10),

$$\inf \mathcal{F}_{\mu,T} = \inf_\rho\big[\big(\inf \mathcal{F}^{\text{can}}_{\rho,T}\big) - \mu\rho\big]. \tag{34}$$

The previous steps have produced energy expressions for the canonical infimum with fixed $\rho$ and $T$. We use these to plot $\big(\inf \mathcal{F}^{\text{can}}_{\rho,T}\big) - \mu_c\rho$ in FIG. 3, where

$$\frac{\mu_c}{8\pi} = 2\rho_{\text{fc}}a - 0.226T^2a^2 + o(T^2a^2). \tag{35}$$

By (34), the derivative of the (red) convex hull of the energy curve at $\rho$ is $\mu - \mu_c$, where $\rho$ is the density of the

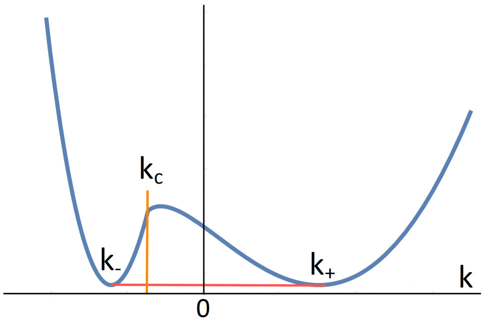


FIG. 3: A plot of $\left(\inf \mathcal{F}^{\text{can}}_{\rho,T}\right) - \mu_{\text{c}}\rho$ as a function of $k$, where $\rho - \rho_{\text{fc}} = \frac{k}{8\pi}T^2a$. The two minima are $k_- = -2.23$ and $k_+ = 3.04$, and the critical value (shown in orange) is $k_{\text{c}} = -1.28$. The energy curve is not convex; the red line indicates the convex hull of the curve.

minimizer of $\mathcal{F}_{\mu,T}$. This way, a grand canonical $\mu$ defines a canonical $\rho(\mu)$. For $\mu < \mu_{\text{c}}$, $\rho(\mu)$ is below $\rho_{\text{c}}$ and hence $\rho_0 = 0$. As we increase to $\mu > \mu_{\text{c}}$, $\rho(\mu)$ jumps across $\rho_{\text{c}}$, and so $\rho_0 > 0$. We have a jump in density at the critical point and conclude that this is a first-order phase transition.

To relate this to the canonical case: we have *coexistence* of the two phases ($\rho_0 = 0$ and $\rho_0 > 0$) for $\rho$ between the two values defined by $k_\pm$. Hence one could say that the system displays BEC for $\rho \geq \rho_{\text{fc}} + \frac{k_-}{8\pi}T^2a$.

□

*Remark.* The analysis above is for $T \approx T_{\text{fc}}$. However, the energy expansions can easily be adapted to lower temperatures. A crucial difference is that the parameter $\rho_0 a/T$ (for example present in (26) through $\rho_0\widehat{Vw}(p)/T$) has to be treated differently. Above, it is of order $Ta^2 \ll 1$, but as $T \to 0$, it will tend to infinity.

To highlight one interesting result for $T \to 0$: we can expand the ground state energy as

$$4\pi a\rho^2 + \frac{512}{15}\sqrt{\pi}(\rho a)^{5/2} + o((\rho a)^{5/2}), \qquad (36)$$

which contains the well-known Lee–Huang–Yang second-order term [16]. This further underlines the accuracy of our model.

*Conclusion and discussion.* We have derived an expression for the critical temperature of weakly-interacting translational-invariant Bose gas in a variational model. The model is conceptually simple, applies to a general class of potentials, and the calculated constant agrees better with numerical predictions than earlier approaches.

The model does produce certain unphysical results, such as a first-order phase transition. It also predicts the occurrence of BEC in 1 and 2 dimensions, which is excluded by the Mermin–Wagner–Hohenberg theorem. These drawbacks are shared with Lee and Yang's work on the hard-core Bose gas [17], and in principle any analysis relying on Bogoliubov's original approach.

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# Paper I

**The Bogoliubov free energy functional I.
Existence of minimizers and phase diagram**

# THE BOGOLIUBOV FREE ENERGY FUNCTIONAL I. EXISTENCE OF MINIMIZERS AND PHASE DIAGRAM

MARCIN NAPIÓRKOWSKI, ROBIN REUVERS, AND JAN PHILIP SOLOVEJ

Abstract. The Bogoliubov free energy functional is analysed. The functional serves as a model of a translation-invariant Bose gas at positive temperature. We prove the existence of minimizers in the case of repulsive interactions given by a sufficiently regular two-body potential. Furthermore, we prove existence of a phase transition in this model and provide its phase diagram.

Contents



## 1. Introduction

Almost all work in the field of interacting Bose gases has its genesis in Bogoliubov's seminal 1947 paper [4]. In this work, Bogoliubov proposed

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an approximate theory of interacting bosons in an attempt to explain the superfluid properties of liquid Helium. Since then, his model has widely been used to study bosonic many-body systems, particularly in the 1950s and 1960s. Despite being intuitively appealing and undoubtedly correct in many aspects, Bogoliubov's theory lacked a mathematically rigorous understanding.

The experimental success in achieving Bose–Einstein condensation in alkali atoms [7] has renewed the interest in the theoretical description of such systems, and significant progress was made in the mathematical analysis of Bose gases. We refer to [19] for an extensive review. Most of these results concern the ground state energies of different bosonic systems.

While Bogoliubov's theory is very useful in relation to these problems, its primary goal was to determine the excitation spectrum of a Bose gas. Indeed, the structure of the excitation spectrum derived by Bogoliubov allowed him to justify Landau's criterion for superfluidity [16], and thus provided a microscopic theory of this phenomenon. A rigorous justification of Bogoliubov's theory in that context has been established only recently for a large class of bosonic systems within the so-called mean-field limit [27, 12, 18, 8, 21] (see [28] for a recent review).

Our goal (and that of the accompanying paper [23]) is to give a variational formulation of Bogoliubov's theory for bosonic systems at positive and zero temperature. Bogoliubov's original approximation consists in adapting the Hamiltonian so that it is quadratic in creation and annihilation operators. We know that ground states or Gibbs states of such Hamiltonians are quasi-free or coherent states. Here, we turn Bogoliubov's theory around and vary over Gaussian states (which include the aforementioned classes of states), whilst retaining the full Hamiltonian. This gives the variational model that we will study in this paper (see Appendix A for relevant definitions and a derivation).

The hope is that our family of states captures important physical aspects of the system; they have for example been used as trial states in establishing the correct asymptotic bounds on the ground state energy of Bose gases [29, 9, 11].

The Bogoliubov variational theory can be seen as the bosonic counterpart of Hartree–Fock theory for Fermi gases. More precisely, it is similar to generalized Hartree–Fock theory, which includes the Bardeen–Cooper–Schrieffer (BCS) trial states and is often called Hartree–Fock–Bogoliubov theory. In HFB theory the trial states are quasi-free states on a fermionic Fock space (see [2] for details).

HFB theory is a widely used tool for understanding fermionic many-body quantum systems. One of the most prominent examples related to this approach is the model of superconductivity that is based on the BCS functional. This model and the related BCS gap equation have been studied both from the physical and mathematical point of view (see e.g. [10, 13, 14]).

In this paper, we are interested in the bosonic counterpart of the BCS functional, or, more precisely, to the BCS functional with the direct and exchange terms included (as discussed in [5]).

Concretely, we want to analyse the model defined by the *Bogoliubov free energy functional* $\mathcal{F}$ given by

$$\begin{aligned}\mathcal{F}(\gamma,\alpha,\rho_0) = (2\pi)^{-3}\int_{\mathbb{R}^3} p^2\gamma(p)dp - \mu\rho - TS(\gamma,\alpha) + \frac{\widehat{V}(0)}{2}\rho^2 \\ + \frac{1}{2}(2\pi)^{-6}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\widehat{V}(p-q)\left(\alpha(p)\alpha(q)+\gamma(p)\gamma(q)\right)dpdq \\ + \rho_0(2\pi)^{-3}\int_{\mathbb{R}^3}\widehat{V}(p)\left(\gamma(p)+\alpha(p)\right)dp,\end{aligned} \tag{1.1}$$

which is the free energy expectation value in a quasi-free state (see Appendix A for a derivation). Here, $\rho$ denotes the density of the system and

$$\rho = \rho_0 + (2\pi)^{-3}\int_{\mathbb{R}^3}\gamma(p)dp =: \rho_0 + \rho_\gamma.$$

The entropy $S(\gamma,\alpha)$ is

$$\begin{aligned}S(\gamma,\alpha) = \quad (2\pi)^{-3}\int_{\mathbb{R}^3} s(\gamma(p),\alpha(p))dp \quad = \quad (2\pi)^{-3}\int_{\mathbb{R}^3} s(\beta(p))dp \\ = (2\pi)^{-3}\int_{\mathbb{R}^3}\left[\left(\beta(p)+\frac{1}{2}\right)\ln\left(\beta(p)+\frac{1}{2}\right) - \left(\beta(p)-\frac{1}{2}\right)\ln\left(\beta(p)-\frac{1}{2}\right)\right]dp,\end{aligned}$$

where

$$\beta(p) := \sqrt{\left(\frac{1}{2}+\gamma(p)\right)^2 - \alpha(p)^2}.$$

The functional is defined on the domain $\mathcal{D}$ given by

$$\mathcal{D} = \{(\gamma,\alpha,\rho_0) | \gamma\in L^1((1+p^2)dp), \gamma(p)\geq 0, \alpha(p)^2\leq\gamma(p)(1+\gamma(p)), \rho_0\geq 0\}.$$

This set-up describes the grand canonical free energy of a homogeneous Bose gas at temperature $T\geq 0$ and chemical potential $\mu\in\mathbb{R}$ in the thermodynamic limit. The particles interact through a repulsive radial two-body potential $V(x)$. Its Fourier transform is denoted by $\widehat{V}(p)$ and is given by

$$\widehat{V}(p) = \int_{\mathbb{R}^3} e^{-ipx}V(x)dx.$$

The function $\gamma\in L^1((1+p^2)dp)$ describes the momentum distribution of the particles in the system. Since the total density equals $\rho = \rho_0 + (2\pi)^{-3}\int_{\mathbb{R}^3}\gamma(p)dp$, it follows that a non-negative $\rho_0$ can be seen as the macroscopic occupation of the state of momentum zero and is therefore interpreted as the density of the Bose–Einstein condensate fraction.

Finally, the function $\alpha(p)$ describes pairing in the system and its non-vanishing value can therefore be interpreted as the presence of off-diagonal long-range order (ODLRO) and the macroscopic coherence related to superfluidity.

To the best of our knowledge, this functional appeared for the first time in the literature in the 1976 paper by Critchley and Solomon [6]. Surprisingly, however, this functional has never been analysed - neither from a mathematical nor a physical point of view. This is probably due to its complexity.

Only various simplified versions of this functional have been studied in the literature (see [32] for an extensive review). Our goal is to fill this gap and provide an analysis of the full functional.

Our work is divided into two parts. In this part, we consider the existence and general properties of equilibrium states of this model. According to statistical mechanics, the equilibrium state corresponding to temperature $T$ and chemical potential $\mu$ is given by the minimizer of (1.1). The free energy is therefore

$$F(T,\mu) = \inf_{(\gamma,\alpha,\rho_0)\in\mathcal{D}} \mathcal{F}(\gamma,\alpha,\rho_0). \tag{1.2}$$

The physical information about the system at a given $T$ and $\mu$ is thus encoded in the structure of the minimizers. For example, a minimizer with $\gamma \equiv 0$ and $\rho_0 > 0$ corresponds to pure Bose–Einstein Condensation; non-vanishing $\alpha$ signifies ODLRO. Hence, any further analysis of the model relies on the well-posedness of the minimization problem (1.2), which we address first. Knowledge about the minimizers for different $(T,\mu)$ then leads to a phase diagram. We will also discuss the relation between Bose–Einstein condensation and superfluidity in translation-invariant systems (see [3] for a historical overview on this topic). Our results are stated in the next section.

In the second part of this work [23], we analyse the functional in the *dilute* (or *low density*) limit. Although Bogoliubov's primary goal was to provide a description for liquid helium, which is a strongly interacting system, it is generally agreed that his theory is more suitable to describe dilute (hence weakly-interacting) systems. Here, low density means that the mean interparticle distance $\rho^{-1/3}$ is much larger than the *scattering length* $a$ of the potential, i.e.

$$\rho^{1/3}a \ll 1.$$

To be able to analyse the dilute limit, we need to consider the *canonical* counterpart of (1.1) at fixed density $\rho$ given by

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) &= (2\pi)^{-3}\int_{\mathbb{R}^3} p^2\gamma(p)dp - TS(\gamma,\alpha) + \frac{\widehat{V}(0)}{2}\rho^2 \\ &\quad + \rho_0(2\pi)^{-3}\int_{\mathbb{R}^3}\widehat{V}(p)\left(\gamma(p)+\alpha(p)\right)dp \\ &\quad + \frac{1}{2}(2\pi)^{-6}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\widehat{V}(p-q)\left(\alpha(p)\alpha(q)+\gamma(p)\gamma(q)\right)dpdq,\end{aligned} \tag{1.3}$$

with $\rho_0 = \rho - \rho_\gamma$. The canonical minimization problem is

$$\begin{aligned}F^{\mathrm{can}}(T,\rho) &= \inf\{\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0=\rho-\rho_\gamma) \mid (\gamma,\alpha,\rho_0=\rho-\rho_\gamma)\in\mathcal{D}\} \\ &= \min\{f(\rho,\rho_0) \mid 0\le\rho_0\le\rho\},\end{aligned} \tag{1.4}$$

where

$$f(\rho,\rho_0) = \inf\{\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) \mid (\gamma,\alpha,\rho_0)\in\mathcal{D}, \rho_\gamma = \rho-\rho_0\}.$$

Strictly speaking, this is not really a canonical formulation: it is only the expectation value of the number of particles that we fix. We will nevertheless describe this energy as canonical. The function $F(T, \mu)$ as a function of $\mu$ is the Legendre transform of the function $F^{\mathrm{can}}(T, \rho)$ as a function of $\rho$.

Having given a proper meaning to the notion of diluteness, one can now ask different questions regarding the low density limit. One particularly interesting problem is how interactions influence the critical temperature (i.e. the temperature of the phase transition between the condensed and non-condensed phase) in a weakly-interacting Bose gas. It is nowadays agreed that the transition temperature should change linearly in $a$, that is

$$\frac{\Delta T_{\mathrm{c}}}{T_{\mathrm{fc}}} \approx c\rho^{1/3}a$$

with $c > 0$. Here $\Delta T_{\mathrm{c}} = T_{\mathrm{c}} - T_{\mathrm{fc}}$, where $T_{\mathrm{c}}$ is the critical temperature in the interacting model and $T_{\mathrm{fc}} = c_0\rho^{2/3}$ is the critical temperature in the non-interacting (ideal) Bose gas.

The results for this model confirm this prediction: in the accompanying paper [23] we prove that

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)),$$

where $\nu = \widehat{V}(0)/a$ and $h_1(8\pi) = 1.49$. This result is in close agreement with numerics: Monte Carlo methods suggest [1, 15, 24] that $c \approx 1.32$. In general $\nu > 8\pi$. It is generally believed, but not rigorously established, that the Bogoliubov model is a good approximation if $\nu$ is replaced by $8\pi$.

Another issue is the asymptotic formula for the free energy (see [26, 31] for the only rigorous results starting from the full many-body problem). In [23], we provide formulas for the free energy of a dilute Bose gas in different regions which correspond to very low ($\rho a/T \gg 1$), fairly low ($\rho a/T \sim O(1)$) and moderate ($\rho a/T \ll 1$) temperatures. In particular, if we let $\nu \to 8\pi$, for very low temperatures we reproduce the well-known Lee–Huang–Yang formula

$$\lim_{T\to 0} F^{\mathrm{can}}(T, \rho) = 4\pi a\rho^2 + \frac{512}{15}\sqrt{\pi}(\rho a)^{5/2} + o(\rho a)^{5/2}.$$

For the reader's convenience, the main results of [23] are also stated in the next section.

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## 2. Main results and sketch of proof

Let us now state the main results of this paper. Throughout this article, we assume that the two-body interaction potential and its Fourier transform are radial functions that satisfy

$$V \geq 0, \quad \widehat{V} \geq 0, \quad V \not\equiv 0. \tag{2.1}$$

Moreover, we assume that

$$\widehat{V} \in C^1(\mathbb{R}^3),\ \widehat{V} \in L^1(\mathbb{R}^3),\ \|\widehat{V}\|_\infty < \infty,\ \|\nabla\widehat{V}\|_2 < \infty,\ \|\nabla\widehat{V}\|_\infty < \infty. \tag{2.2}$$

2.1. **Existence of minimizers.** We start by providing the existence results that form the basis of any further analysis.

**Theorem 1** (Existence of grand canonical minimizers for $T > 0$)**.** *Let $T > 0$. Assume the interaction potential is a radial function that satisfies* (2.1) *and* (2.2)*. Then there exists a minimizer for the Bogoliubov free energy functional* (1.1) *defined on $\mathcal{D}$.*

It turns out that we need to assume some additional regularity on the interaction potential to prove a similar statement for $T = 0$ .

**Theorem 2** (Existence of grand canonical minimizers for $T = 0$)**.** *Assume the interaction potential fulfils the assumptions of Theorem 1. If we assume in addition that $\widehat{V} \in C^3(\mathbb{R}^3)$ and that all derivatives of $\widehat{V}$ up to third order are bounded, then there exists a minimizer for the Bogoliubov free energy functional* (1.1) *defined on $\mathcal{D}$ for $T = 0$.*

We expect that our assumptions on the interaction potential are far from optimal. A natural direction for further research would be to try to extend the above results to the case of more singular potentials. In the fermionic case, the existence of minimizers for the HFB functional with Newtonian interaction turned out to be surprisingly difficult to prove [17].

*Remark* 3. We would like to stress that the minimizers need not be unique. In fact, a detailed analysis of the dilute limit case in [23] shows that there exist combinations of $\mu$ and $T$ for which the problem (1.2) has two minimizers with two different densities.

We have analogous results in the canonical setting.

**Theorem 4** (Existence of canonical minimizers for $T > 0$)**.** *Let $T > 0$. Assume the interaction potential is a radial function that satisfies* (2.1) *and* (2.2)*. Then the variational problem* (1.4) *admits a minimizer.*

**Theorem 5** (Existence of canonical minimizers for $T = 0$)**.** *Assume the interaction potential fulfils the assumptions of Theorem 4. If we assume in addition that $\widehat{V} \in C^3(\mathbb{R}^3)$ and that all derivatives of $\widehat{V}$ up to third order are bounded, then there exists a minimizer for the canonical minimization problem* (1.4) *at $T = 0$.*

A nice property that follows from the proof of Theorems 2 and 5 is the following fact.

**Corollary 6** (Structure of $T = 0$ minimizers)**.** *Minimizers for the canonical and grand canonical problem at $T = 0$ are pure quasi-free states.*

Note that this result is not obvious. It is well known that pure quasi-free states are minimizers for quadratic Hamiltonians. Our model, however, involves also higher order terms.

2.2. **Existence and structure of phase transition.** We now analyse the structure of the minimizers. Our first result shows that Bose–Einstein condensation and superfluidity are equivalent within our models.

**Theorem 7** (Equivalence of BEC and superfluidity)**.** *Let* $(\gamma, \alpha, \rho_0)$ *be a minimizing triple for either* (1.1) *or* (1.3)*. Then*

$$\rho_0 = 0 \Longleftrightarrow \alpha \equiv 0.$$

Hence, there exists only one kind of phase transition within our model. The next results show that this phase transition indeed exists.

**Theorem 8** (Existence of grand canonical phase transition)**.** *Let* $\mu > 0$*. Then there exist temperatures* $0 < T_1 < T_2$ *such that a minimizing triple* $(\gamma, \alpha, \rho_0)$ *of* (1.2) *satisfies*

(1) $\rho_0 = 0$ *for* $T \geq T_2$
(2) $\rho_0 > 0$ *for* $0 \leq T \leq T_1$.

**Theorem 9** (Existence of canonical phase transition)**.** *For fixed* $\rho > 0$ *there exist temperatures* $0 < T_3 < T_4$ *such that a minimizing triple* $(\gamma, \alpha, \rho_0)$ *of* (1.4) *satisfies*

(1) $\rho_0 = 0$ *for* $T \geq T_4$
(2) $\rho_0 > 0$ *for* $0 \leq T \leq T_3$.

*Remark* 10. All the statements remain true in one and two dimensions.

2.3. **Grand canonical phase diagram.** The results stated above together with their proofs allow us to sketch a phase diagram of the system, see Figure 1.

Note that at $T = 0$ and $\mu < 0$ the minimizer corresponds to the vacuum. Also, for negative chemical potentials there is no phase transition in the system.

The area with the lighter shade of blue indicates that we cannot rule out multiple phase transitions with different critical temperatures. This is, however, unexpected. The vanishing of this area as $\mu$ approaches zero from the right is a consequence of the results in [23], which we review next. See, in particular, Theorem 12.

2.4. **Main results of** [23]**.** The main results of [23] hold under several general assumptions. For the following three results, we assume that we are in the dilute limit

$$\rho^{1/3} a \ll 1, \tag{2.3}$$

where $a$ is the scattering length of the potential. Furthermore, we define the constant $C$ by

$$\int \widehat{V} \leq C a^{-2} \qquad \text{and} \qquad \|\partial^n \widehat{V}\|_\infty \leq C a^{n+1} \text{ for } 0 \leq n \leq 3, \tag{2.4}$$

where $\partial^n$ is shorthand for all $n$-th order partial derivatives. With this definition, our estimates depend only on $C$ and not on $a$. Recall $\nu := \widehat{V}(0)/a$.

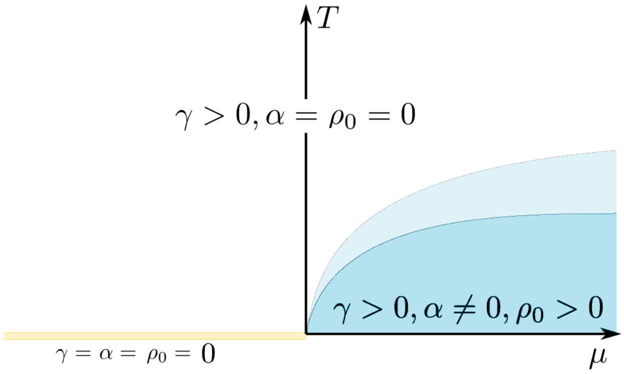


FIGURE 1. The grand canonical phase diagram of the model. No diluteness is assumed. At $\mu \leq 0$ and $T = 0$, all quantities are zero, in particular there is no BEC. Increasing $T$ does not lead to a phase transition, although $\gamma$ becomes non-zero. For $\mu > 0$ fixed and $T = 0$, there is BEC. This remains the case when $T$ increases (darkest region), eventually leading to a phase transition somewhere in the lighter region before we enter the white region where $\rho_0 = 0$.

The following theorems contain information about the critical temperature of the phase transition in the dilute limit.

**Theorem 11** (Canonical critical temperature)**.** *Let* $(\gamma, \alpha, \rho_0)$ *be a minimizing triple of* (1.4) *at temperature* $T$ *and density* $\rho$*. There is a monotone increasing function* $h_1 : (8\pi, \infty) \to \mathbb{R}$ *with* $h_1(\nu) \geq \lim_{\nu \to 8\pi} h_1(\nu) = 1.49$ *such that*

(1) $\rho_0 \neq 0$ *if* $T < T_{\text{fc}} \left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$
(2) $\rho_0 = 0$ *if* $T > T_{\text{fc}} \left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$,

*where* $T_{\text{fc}} = c_0\rho^{2/3}$ *is the critical temperature of the free Bose gas.*

**Theorem 12** (Grand canonical critical temperature)**.** *Let* $(\gamma, \alpha, \rho_0)$ *be a minimizing triple of* (1.2) *at temperature* $T$ *and chemical potential* $\mu$*. There is a function* $h_2 : (8\pi, \infty) \to \mathbb{R}$ *with* $\lim_{\nu \to 8\pi} h_2(\nu) = 0.44$ *such that*

(1) $\rho_0 \neq 0$ *if* $T < \left(\frac{\sqrt{\pi}}{2\zeta(3/2)} \frac{8\pi}{\nu}\right)^{2/3} \left(\frac{\mu}{a}\right)^{2/3} + h_2(\nu)\mu + o(\mu)$
(2) $\rho_0 = 0$ *if* $T > \left(\frac{\sqrt{\pi}}{2\zeta(3/2)} \frac{8\pi}{\nu}\right)^{2/3} \left(\frac{\mu}{a}\right)^{2/3} + h_2(\nu)\mu + o(\mu)$.

We refer to [23] for the proof of these statements.

The second main result of [23] provides an expansion of the canonical free energy (1.4) in the dilute limit. Here, we only state what happens for $\nu = \widehat{V}(0)/a \to 8\pi$. We need to define an integral first:

$$I(s) = (2\pi)^{-3} \int \ln\left(1 - e^{-\sqrt{p^4 + 16\pi p^2 s^2}}\right) dp.$$

*Remark* 13. Let $T_{\text{fc}} = c_0\rho^{2/3}$ be the critical temperature of the free Bose gas, and $\rho_{\text{fc}} = (T/c_0)^{3/2}$ its corresponding critical density. In the limit $\nu \to 8\pi$, the canonical free energy (1.4) can be expanded in the following way.

(1) If $T > T_{\rm fc}\left(1 + 1.49\rho^{1/3}a + o(\rho^{1/3}a)\right)$, then

$$F^{\rm can}(T,\rho) = F_0(T,\rho) + \widehat{V}(0)\rho^2 + O(\rho a)^{5/2},$$

and we have $\rho_\gamma = \rho$, $\rho_0 = 0$ for the minimizer. Here, $F_0(T,\rho)$ is the free energy of the non-interacting gas at density $\rho$ and temperature $T$.

(2) If $T < T_{\rm fc}\left(1 + 1.49\rho^{1/3}a + o(\rho^{1/3}a)\right)$, then

$$\begin{aligned} F^{\rm can}(T,\rho) &= 4\pi a\rho^2 + 4\pi a\rho_{\rm fc}^2 + \frac{512}{15}\sqrt{\pi}(\rho a)^{5/2} \\ &\quad + T^{5/2} I\left(\sqrt{\frac{(\rho-\rho_{\rm fc})a}{T}} + \frac{1}{4\sqrt{\pi}}\sqrt{T}a\right) - 4\sqrt{\pi}T\rho_{\rm fc}a\sqrt{(\rho-\rho_{\rm fc})a} \\ &\quad + o\left(T(\rho a)^{3/2} + (\rho a)^{5/2}\right). \end{aligned}$$

The last expression reduces to the Lee–Huang–Yang formula for $T \ll \rho a$:

$$F^{\rm can}(T,\rho) = 4\pi a\rho^2 + \frac{512}{15}\sqrt{\pi}(\rho a)^{5/2} + o(\rho a)^{5/2}.$$

2.5. **Sketch of proofs and set-up of the paper.** The rest of the paper is devoted to the proofs of the statements described in Subsections 2.1, 2.2 and 2.3.

In Section 3 we provide some general facts that will be useful throughout the paper.

Section 4 contains the proofs of Theorems 1 and 4. Section 5 provides proofs of Theorems 2 and 5.

The proof of the existence of minimizers in our model is harder than in the case of the fermionic BCS functional [13]. The main reason for this is the occurrence of Bose–Einstein Condensation (BEC). Loosely speaking, at sufficiently low temperatures bosons tend to macroscopically occupy the same quantum state. Since in our model the momentum distribution of the particles is described by $\gamma(p)$, this suggests that there is no a priori bound on this function. Therefore, a minimizing sequence could convergence to a measure which could have a singular part that represents the condensate. This scenario, however, has been included in the construction of the functional by introducing the parameter $\rho_0$ that represents the condensate density.

The situation for is simpler for fermions as there is an a priori bound on $\gamma$: the Pauli principle implies that $\gamma \leq 1$.

Let us now present the main ideas behind the proof. We start by reformulating the problem in terms of an auxiliary functional. We show that to prove the main theorem it is enough to prove the existence of a minimizer for the problem

$$F^{\rm aux}(\lambda,\rho_0) = \inf\left\{\mathcal{F}^{\rm aux}(\gamma,\alpha,\rho_0) \;\middle|\; \int \gamma(p)dp = \lambda, (\gamma,\alpha)\in\mathcal{D}'\right\},$$

where

$$\mathcal{F}^{\rm aux} = \mathcal{F} + \mu\rho - \frac{\widehat{V}(0)}{2}\rho^2$$

and

$$\mathcal{D}' = \{(\gamma,\alpha) \mid \gamma \in L^1((1+p^2)dp),\ \gamma(p)\geq 0,\ \alpha(p)^2 \leq \gamma(p)(\gamma(p)+1)\}.$$

We will see below that all terms in $\mathcal{F}$ are bounded on $\mathcal{D}'$.

The advantage of considering a functional for fixed $\rho_0$ is that one obtains joint convexity in $(\gamma, \alpha)$.

To prove the existence of minimizers for the auxiliary problem (which is a constrained minimization problem), we consider the dual problem. We also restrict our functional to the smaller space

$$\mathcal{M}_\kappa = \{(\gamma, \alpha) \in \mathcal{D}' | \gamma(p) \leq \frac{\kappa}{p^2}\}.$$

Note that restricting the domain to $\mathcal{M}_\kappa$ imposes an artificial a priori bound which is used to prove the existence of minimizers for this restricted problem. The idea is then to construct a minimizing sequence of the unrestricted problem out of the minimizers $\gamma_\kappa$ of the restricted problem in the limit $\kappa \to \infty$.

To this end we prove several bounds for the $\gamma_\kappa$'s. These bounds show that the minimizers are uniformly bounded for $p$ such that $|p| \geq p_\kappa$ where $p_\kappa \to 0$ as $\kappa \to \infty$. Thus, physically speaking, we show that if there is condensation, then it can occur only in the $p = 0$ mode.

The last main step is then to show that mass accumulation at $p = 0$ is impossible for a minimizer, since this would increase the energy compared to a solution where the mass would be added to $\rho_0$ from the start.

The proof that we sketched above only works for $T > 0$ since the bounds we mentioned are not uniform in $T$ and deteriorate as $T \to 0$. It turns out that the positive temperature minimizers $(\gamma^T, \alpha^T, \rho_0^T)$ form a uniformly equicontinuous family that is also a minimizing sequence for the $T = 0$ problem. Using the Arzelà–Ascoli theorem one can then extract a limit which turns out to be a minimizer.

The proofs of Theorems 8 and 9 as well as the proof of Theorem 7 and the discussion of the grand canonical phase diagram are provided in Section 6.

As mentioned in the introduction, we provide an introduction to Bogoliubov's variational theory and a derivation of the functional in Appendix A.

## 3. Preliminaries

Let us start with several remarks and bounds which will be used later. Throughout the proofs $C, C_1, ...$ stand for unspecified universal constants.

Recall the notation

$$\beta(p) := \sqrt{(\frac{1}{2} + \gamma(p))^2 - \alpha(p)^2}.$$

Since

$$s(\beta) = -(\beta - \frac{1}{2}) \ln(\beta - \frac{1}{2}) + (\beta + \frac{1}{2}) \ln(\beta + \frac{1}{2})$$

and

$$\frac{\partial s(\beta)}{\partial \beta} = \ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}$$

we have

$$s(\gamma, \alpha) < s(\gamma, 0), \text{ if } \alpha \neq 0. \tag{3.1}$$

Several bounds will rely on the decomposition $\alpha = \alpha_< + \alpha_>$ where $\alpha_< := \alpha\mathbb{1}_{\{\gamma<1\}}$ and $\alpha_> := \alpha\mathbb{1}_{\{\gamma\geq 1\}}$. The condition

$$\alpha^2 \leq \gamma^2 + \gamma \tag{3.2}$$

then implies that $|\alpha_>| \leq \sqrt{2}\gamma$ and $|\alpha_<| \leq \sqrt{2}\sqrt{\gamma}$. Thus using the assumptions on $V$ and $\widehat{V}$ we have

$$\begin{aligned}
\left|\int \widehat{V}(p)\alpha(p)dp\right| &\leq \int\limits_{\{\gamma\geq 1\}} \widehat{V}(p)|\alpha_>(p)|dp + \int\limits_{\{\gamma<1\}} \widehat{V}(p)|\alpha_<(p)|dp \\
&\leq \int\limits_{\{\gamma\geq 1\}} \widehat{V}(p)\sqrt{2}\gamma(p)dp + \int\limits_{\{\gamma<1\}} \widehat{V}(p)\sqrt{2}\sqrt{\gamma(p)}dp \\
&\leq \sqrt{2}\widehat{V}(0)\int\limits_{\{\gamma\geq 1\}} \gamma(p)dp + \sqrt{2}\int\limits_{\{\gamma<1\}} \widehat{V}(p)dp < C(\|\gamma\|_1, \widehat{V}).
\end{aligned} \tag{3.3}$$

Similarly

$$\begin{aligned}
&\iint \widehat{V}(p-q)\alpha(p)\alpha(q)dpdq = \iint \widehat{V}(p-q)\alpha_>(p)\alpha_>(q)dpdq \\
&+ \iint \widehat{V}(p-q)\alpha_<(p)\alpha_<(q)dpdq + 2\iint \widehat{V}(p-q)\alpha_>(p)\alpha_<(q)dpdq \\
&< C(\|\gamma\|_1, \|\widehat{V}\|_1, \|\widehat{V}\|_\infty),
\end{aligned}$$

since

$$\iint \widehat{V}(p-q)\alpha_>(p)\alpha_>(q)dpdq \leq \widehat{V}(0)\left(\int |\alpha_>|\right)^2 \leq 2\widehat{V}(0)\left(\int \gamma\right)^2,$$

$$\begin{aligned}
\iint \widehat{V}(p-q)\alpha_<(p)\alpha_<(q)dpdq &\leq 2\iint \widehat{V}(p-q)\sqrt{\gamma(p)}\sqrt{\gamma(q)}dpdq \\
&\leq \iint \widehat{V}(p-q)(\gamma(p)+\gamma(q))dpdq = 2\left(\int \widehat{V}\right)\left(\int \gamma\right)
\end{aligned}$$

and

$$\iint \widehat{V}(p-q)\alpha_>(p)\alpha_<(q)dpdq \leq 2\iint \widehat{V}(p-q)\gamma(p)dpdq.$$

Obviously

$$\iint \widehat{V}(p-q)\alpha(p)\alpha(q)dpdq = \int V(x)|\check{\alpha}(x)|^2 dx \geq 0. \tag{3.4}$$

Another useful consequence of (3.2) is the lower pointwise bound

$$\gamma + \alpha \geq -\frac{1}{2}. \tag{3.5}$$

For the convolution terms one easily sees that

$$\|\widehat{V} * \gamma\|_\infty \leq \|\widehat{V}\|_\infty \|\gamma\|_1 \leq C(\|\gamma\|_1, \|\widehat{V}\|_1, \|\widehat{V}\|_\infty), \tag{3.6}$$

$$\|\widehat{V} * \alpha\|_\infty \leq \|\widehat{V}\|_\infty \|\alpha_>\|_1 + \|\widehat{V}\|_2 \|\alpha_<\|_2 \leq C\left(\|\gamma\|_1, \|\widehat{V}\|_1, \|\widehat{V}\|_\infty\right). \tag{3.7}$$

We will also use the following lower bound on the free energy of a non-interacting system

$$\begin{aligned}\int p^2\gamma - T\int s(\beta) &\geq \int p^2\gamma_0 - T\int s(\gamma_0, 0)\\ &= T\int \ln\left(1 - e^{\frac{-p^2}{T}}\right) dp > -C,\end{aligned} \tag{3.8}$$

where $\gamma_0 = \left(\exp(p^2/T) - 1\right)^{-1}$. This follows from (3.1) and a direct computation. It follows, in particular, that all terms in $\mathcal{F}$ are bounded on $\mathcal{D}'$.

## 4. Existence of minimizers for $T > 0$

4.1. **Reduction to the auxiliary problem.** Let us introduce the auxiliary free energy functional defined by

$$\begin{aligned}\mathcal{F}^{\mathrm{aux}}(\gamma, \alpha, \rho_0) = &\int p^2\gamma(p)dp - T\int s(\gamma(p), \alpha(p))dp\\ &+ \rho_0 \int \widehat{V}(p)(\gamma(p) + \alpha(p))dp\\ &+ \frac{1}{2}\iint \widehat{V}(p-q)(\gamma(p)\gamma(q) + \alpha(p)\alpha(q))dpdq.\end{aligned}$$

For notational simplicity, we have absorbed $(2\pi)^{-3}$ in every integral compared to (1.1), so that the measure is really $(2\pi)^{-3}dp$. We will use the same convention for the real space measure $dx$, but not for one-dimensional measures $dt$ or $ds$. We introduce the following minimization problem

$$F^{\mathrm{aux}}(\lambda, \rho_0) = \inf\left\{\mathcal{F}^{\mathrm{aux}}(\gamma, \alpha, \rho_0) \;\middle|\; \int \gamma(p)dp = \lambda, (\gamma, \alpha) \in \mathcal{D}'\right\}, \tag{4.1}$$

where

$$\mathcal{D}' = \{(\gamma, \alpha) \mid \gamma \in L^1((1 + p^2)dp),\ \gamma(p) \geq 0,\ \alpha(p)^2 \leq \gamma(p)(\gamma(p) + 1)\}.$$

**Proposition 14.** *The existence of a minimizer for the auxiliary problem* (4.1) *implies the existence of minimizers for the grand canonical problem* (1.2) *and canonical problem* (1.4).

To prove this proposition we will need two lemmas.

**Lemma 15.** *The functional $\mathcal{F}^{\mathrm{aux}}$ is jointly (strictly) convex in $(\gamma, \alpha)$ and $\mathcal{D}'$ is a convex set.*

*Proof.* First notice that the Hessian of $-s(\gamma, \alpha)$ regarded as a function of $\gamma$ and $\alpha$ is positive definite. Since $V \geq 0$ the expressions $\iint \widehat{V}(p - q)\gamma(p)\gamma(q)dpdq$ and $\iint \widehat{V}(p-q)\alpha(p)\alpha(q)dpdq$ are convex in $\gamma$ and $\alpha$ respectively. It follows that $\mathcal{F}^{\mathrm{aux}}$ as a sum of jointly convex functions is jointly convex in $(\gamma, \alpha)$. Convexity of $\mathcal{D}'$ follows from a simple calculation. □

**Lemma 16.** *The function $F^{\mathrm{aux}}(\lambda, \rho_0)$ is convex in $\lambda$, concave in $\rho_0$ and continuous as a function of two variables.*

*Proof. Convexity in $\lambda$.* This is straightforward from the convexity in Lemma 15.

*Concavity in $\rho_0$.* This follows from the fact that minimization of a functional that is linear in a variable yields a concave function in that variable.

*Continuity of $F^{\text{aux}}(\lambda, \rho_0)$.* Define

$$\begin{aligned}\tilde{\mathcal{F}}^{\text{aux}}(\gamma, \alpha, \rho_0) = &\int p^2 \gamma(p) dp - TS(\gamma, \alpha) \\ &+ \frac{1}{2} \iint \widehat{V}(p-q)(\gamma(p) + \rho_0 \delta_0)(\gamma(q) + \rho_0 \delta_0) dp dq \\ &+ \frac{1}{2} \iint \widehat{V}(p-q)(\alpha(p) + \rho_0 \delta_0)(\alpha(q) + \rho_0 \delta_0) dp dq,\end{aligned}$$

where $\delta_0$ is the Dirac Delta function. Then as before $\tilde{\mathcal{F}}^{\text{aux}}$ is jointly convex in $(\gamma, \alpha, \rho_0)$. Then

$$\tilde{F}^{\text{aux}}(\lambda, \rho_0) = \inf_{\substack{(\gamma,\alpha)\in\mathcal{D}' \\ \int \gamma = \lambda}} \tilde{\mathcal{F}}^{\text{aux}}(\gamma, \alpha, \rho_0)$$

is jointly convex in $\lambda$ and $\rho_0$ and hence continuous on $(0, \infty) \times (0, \infty)$.

We now consider the points of the form $(\lambda^*, 0)$ with $\lambda^* > 0$ on the boundary. By convexity, we have

$$\lim_{(\lambda,\rho_0)\to(\lambda^*,0)} \tilde{F}^{\text{aux}}(\lambda, \rho_0) \leq \tilde{F}^{\text{aux}}(\lambda^*, 0),$$

where the limit on the left is independent of the way we approach the boundary point. To show the opposite inequality, note that we can use approximate minimizers for $(\lambda^*, \rho_0)$ as trial states for $(\lambda^*, 0)$ by plugging them in with $\rho_0 = 0$. In the limit $\rho_0 \to 0$, these trial states approximate the limit above, proving continuity at this boundary.

The boundary $(0, \rho_0^*)$ with $\rho_0^* \geq 0$ can be treated in the same way, where we use the estimates from Section 3 to estimate the terms involving $\gamma$ and $\alpha$ as $\lambda \to 0$.

It follows that $F^{\text{aux}}(\lambda, \rho_0) = \tilde{F}^{\text{aux}}(\lambda, \rho_0) - \rho_0^2 \widehat{V}(0)$ is continuous as well. □

*Proof of Proposition 14.* As $F^{\text{aux}}$ is continuous we conclude that $F^{\text{aux}}(\rho - \rho_0, \rho_0)$ has a minimizing $\rho_0$ satisfying $0 \leq \rho_0 \leq \rho$. The problem (1.4) is then minimized for this $\rho_0$ and the $(\gamma, \alpha)$ that minimizes (4.1).

In the grand canonical case, by the definitions of $F(T, \mu)$ and $F^{\text{aux}}(\lambda, \rho_0)$ we have

$$F(T, \mu) = \inf_{\lambda,\rho_0} \left[ F^{\text{aux}}(\lambda, \rho_0) - \mu(\lambda + \rho_0) + \frac{\widehat{V}(0)}{2}(\lambda + \rho_0)^2 \right]. \tag{4.2}$$

Using (3.5) and (3.8) we see that

$$F^{\text{aux}}(\lambda, \rho_0) \geq -C_1 \rho_0 - C_2.$$

Thus there exists an infimum in (4.2) that (by continuity of the underlying function) is also a minimum. For given $\mu$ and $T$ we can find the corresponding minimizing $\lambda$ and $\rho_0$ and thus by the assumption of the existence of a minimizer for $\mathcal{F}^{\text{aux}}$ we find a minimizer for $\mathcal{F}(\gamma, \alpha, \rho_0)$. □

4.2. **The dual auxiliary problem.** We now proceed to the proof of the existence of a minimizer for the auxiliary problem (4.1). This is a problem of constrained minimization. By Lemma 16 the function $F^{\text{aux}}(\lambda, \rho_0)$ is convex in $\lambda$. Thus the constrained minimization problem (4.1) is equivalent to the unconstrained *dual auxiliary problem*:

$$\widehat{F}^{\text{aux}}(\delta, \rho_0) := \inf_{(\gamma,\alpha)\in\mathcal{D}'} \left\{ \mathcal{F}^{\text{aux}}(\gamma, \alpha, \rho_0) - \delta \int \gamma \right\} =: \inf_{(\gamma,\alpha)\in\mathcal{D}'} \mathcal{F}^{\text{aux}}_{\delta}(\gamma, \alpha, \rho_0), \tag{4.3}$$

where $\delta$ is chosen as the slope of a supporting hyperplane at $\lambda$ for the convex function $\lambda \mapsto F^{\text{aux}}(\lambda, \rho_0)$.

Before we move on let us state a simple property of the dual auxiliary functional.

**Lemma 17** (Radiality of minimizers)**.** *A minimizer $(\gamma, \alpha)$ of* (4.3) *(and therefore* (4.1)*), if it exists, is radial:*

$$(\gamma(Rp), \alpha(Rp)) = (\gamma(p), \alpha(p)) \text{ for any } R \in SO(3).$$

*Proof.* The strict convexity in Lemma 15 implies that a minimizer of (4.1) (and hence (4.3)) is unique assuming it exists. The result follows since $p \mapsto (\gamma(Rp), \alpha(Rp))$ is a minimizer if $p \mapsto (\gamma(p), \alpha(p))$ is. □

**Lemma 18** (Coercivity)**.** *Let $\delta \in \mathbb{R}$. The functional $\mathcal{F}^{\text{aux}}_{\delta}(\gamma, \alpha, \rho_0)$ is coercive in $\gamma$, i.e. there exist constants $C_1, c_2, c_3 > 0$ depending on $T$, $\rho$, $\delta$ and $V$ such that for $0 \le \rho_0 \le \rho$*

$$\mathcal{F}^{\text{aux}}(\gamma, \alpha, \rho_0) - \delta \int \gamma \ge -C_1 + c_2 \int p^2 \gamma(p) dp + c_3 \int \gamma.$$

*In particular, any minimizing sequence $\gamma_n$ is bounded in $L^1(\mathbb{R}^3, dp)$ and $L^1(\mathbb{R}^3, p^2 dp)$. Moreover, $c_2$ and $c_3$ are independent of $T$ and $C_1$ is bounded as $T$ goes to zero.*

*Proof.* By (3.5), (3.1) and (3.4) it follows that

$$\begin{aligned} \mathcal{F}^{\text{aux}}(\gamma, \alpha, \rho_0) - \delta \int \gamma \ge{}& \frac{1}{2} \int p^2 \gamma(p) dp - T \int s(\gamma, 0) dp - \frac{1}{2}\rho_0 \int \widehat{V}(p) dp \\ &+ \frac{1}{8} \int p^2 \gamma(p) dp + \frac{1}{2} \int (\frac{3}{4}p^2 - 2\delta)\gamma(p) dp + \frac{1}{2} \iint \widehat{V}(p-q)\gamma(p)\gamma(q) dp dq. \end{aligned} \tag{4.4}$$

The first two terms on the right-hand side of (4.4) are bounded from below by a constant $C_T$ that depends only on $T$ in the same way as in (3.8). It thus remains to bound from below the last two terms in (4.4). To this end we split $\gamma$ into two parts: $\gamma_{\text{in}}$ with support in $\{p | \frac{3}{4}p^2 - 2\delta \le \varepsilon_\delta\}$ and $\gamma_{\text{out}}$ with support in $\{p | \frac{3}{4}p^2 - 2\delta > \varepsilon_\delta\}$, where some $\varepsilon_\delta > 2|\delta|$ is chosen. Then

$$\begin{aligned} \frac{1}{2} \int (\frac{3}{4}p^2 - 2\delta)\gamma(p) dp + \frac{1}{2} \iint \widehat{V}(p-q)\gamma(p)\gamma(q) dp dq \ge{}& \frac{\varepsilon_\delta}{2} \int \gamma_{\text{out}} - \delta \int \gamma_{\text{in}} \\ &+ \frac{1}{2} \iint \widehat{V}(p-q)\gamma_{\text{in}}(p)\gamma_{\text{in}}(q) dp dq, \end{aligned}$$

where we have left out the other positive terms coming from the convolution. Since

$$|\nabla\check{\gamma}_{\rm in}(x)| \leq \int |p|\gamma_{\rm in}(p)dp,$$

we have

$$|\nabla\check{\gamma}_{\rm in}(x)| \leq C_\delta \check{\gamma}_{\rm in}(0),$$

and hence $\check{\gamma}_{\rm in}(x) \geq \frac{1}{2}\check{\gamma}_{\rm in}(0)$ for sufficiently small $|x|$ depending only on $\delta$. Also, by continuity, we have $V(x) > \frac{1}{2}V(0)$ for sufficiently small $|x|$. Let $B_\delta$ denote the ball where both these conditions are fulfilled. Note that such a ball can be chosen independently of $\gamma$. It follows that

$$\frac{1}{2}\iint \widehat{V}(p-q)\gamma_{\rm in}(p)\gamma_{\rm in}(q)dpdq \geq \frac{|B_\delta|}{8}V(0)\left(\int \gamma_{\rm in}\right)^2.$$

Together with the previous estimate this implies that

$$\mathcal{F}_\delta^{\rm aux}(\gamma,\alpha,\rho_0) \geq -C_T + \frac{1}{8}\int p^2\gamma(p)dp + \frac{\varepsilon_\delta}{2}\int\gamma_{\rm out} - \delta\int\gamma_{\rm in} + C_{\delta,V}\left(\int\gamma_{\rm in}\right)^2.$$

Since $\int\gamma = \int\gamma_{\rm in} + \int\gamma_{\rm out}$ the lemma follows. □

Unfortunately, since $L^1$ is not reflexive, the boundedness of the minimizing sequence (which follows from the lemma above) is not enough to extract a weakly converging subsequence. We therefore consider the *restricted dual auxiliary problem*, by which we mean the problem of finding

$$\widehat{F}_\kappa^{\rm aux}(\delta,\rho_0) = \inf_{(\gamma,\alpha)\in\mathcal{M}_\kappa} \mathcal{F}_\delta^{\rm aux}(\gamma,\alpha,\rho_0), \tag{4.5}$$

where $\kappa \geq 1$ and

$$\mathcal{M}_\kappa = \{(\gamma,\alpha)\in\mathcal{D}' | \gamma(p) \leq \frac{\kappa}{p^2}\}. \tag{4.6}$$

**Proposition 19** (Existence of minimizers for the restricted problem)**.** *There exists a minimizer for the restricted problem* (4.5).

*Proof. Step 1.* Let $(\gamma_n,\alpha_n)$ be a minimizing sequence in $\mathcal{M}_\kappa$. It follows from Lemma 18 that $\|\gamma_n\|_1 < C$ and that $\int p^2\gamma_n(p)dp < C$ for some constant $C$ depending on $T, V$ and $\delta$, but independent of $n$.

*Step 2.* We claim that $(\gamma_n,\alpha_n)$ is a bounded sequence in $L^s(\mathbb{R}^3)\times L^s(\mathbb{R}^3)$ for $s\in(\frac{6}{5},\frac{3}{2})$. To this end consider the set

$$\mathcal{A}_n = \{p \,|\, \gamma_n(p) > 1\}.$$

Since

$$\int_{\mathbb{R}^3}\gamma_n \geq \int_{\mathcal{A}_n}\gamma_n \geq |\mathcal{A}_n|,$$

the condition $\|\gamma_n\|_1 < C$ implies that for any $n$ we have $|\mathcal{A}_n| < C$. Furthermore for $s\in(1,\frac{3}{2})$ we have

$$\|\gamma_n\|_s^s = \int_{\mathbb{R}^3\setminus\mathcal{A}_n}\gamma_n^s + \int_{\mathcal{A}_n}\gamma_n^s \leq \int_{\mathbb{R}^3\setminus\mathcal{A}_n}\gamma_n + \int_{\mathcal{A}_n}\frac{\kappa^s}{p^{2s}}dp < C, \tag{4.7}$$

where we used the restriction imposed by (4.6). Indeed, by the previous step we have $\int_{\mathbb{R}^3\setminus\mathcal{A}_n}\gamma_n < C$. To bound the last term we use the fact that $|\mathcal{A}_n| < C$. Then

$$\int_{\mathcal{A}_n}\frac{\kappa^s}{p^{2s}}dp = \int_{\mathcal{A}_n\cap B(0,1)}\frac{\kappa^s}{p^{2s}}dp + \int_{\mathcal{A}_n\setminus B(0,1)}\frac{\kappa^s}{p^{2s}}dp \le \int_{B(0,1)}\frac{\kappa^s}{p^{2s}}dp + |\mathcal{A}_n|\kappa^s,$$

which is bounded uniformly in $n$ for $s < \frac{3}{2}$. Here, $B(0,1)$ denotes the unit ball centred at the origin. Let us now consider the bound on $\|\alpha_n\|_s$. Using (3.2) we have

$$\|\alpha_n\|_s^s = \int_{\mathbb{R}^3\setminus\mathcal{A}_n}|\alpha_n|^s + \int_{\mathcal{A}_n}|\alpha_n|^s \le 2^{\frac{s}{2}}\int_{\mathbb{R}^3\setminus\mathcal{A}_n}\sqrt{\gamma_n}^s + 2^{\frac{s}{2}}\int_{\mathcal{A}_n}\gamma_n^s.$$

By (4.7), the last term is bounded uniformly in $n$. To bound the other term, notice that by the uniform bound $\int p^2\gamma_n(p)dp < C$ it follows from Hölder's inequality that

$$\begin{aligned}\int_{\mathbb{R}^3\setminus\mathcal{A}_n}\gamma_n^{\frac{s}{2}} = &\int_{(\mathbb{R}^3\setminus\mathcal{A}_n)\cap B(0,1)}\gamma_n^{\frac{s}{2}} + \int_{(\mathbb{R}^3\setminus\mathcal{A}_n)\setminus B(0,1)}\gamma_n^{\frac{s}{2}}\\ &\le C + \int_{(\mathbb{R}^3\setminus\mathcal{A}_n)\setminus B(0,1)}\frac{(p^2\gamma_n)^{\frac{s}{2}}}{p^s}dp\\ &\le C + \left(\int_{(\mathbb{R}^3\setminus\mathcal{A}_n)\setminus B(0,1)}p^2\gamma_n dp\right)^{\frac{s}{2}}\left(\int_{(\mathbb{R}^3\setminus\mathcal{A}_n)\setminus B(0,1)}p^{\frac{2s}{s-2}}dp\right)^{\frac{2-s}{2}}.\end{aligned}$$

For $\frac{6}{5} < q < \frac{3}{2}$ a uniform bound follows.

*Step 3.* By the previous step, we can find a subsequence that converges weakly, i.e. there exist $(\tilde{\gamma},\tilde{\alpha}) \in L^s(\mathbb{R}^3)\times L^s(\mathbb{R}^3)$ such that $(\gamma_n,\alpha_n) \rightharpoonup (\tilde{\gamma},\tilde{\alpha})$ for $s \in (\frac{6}{5},\frac{3}{2})$. Using Mazur's Lemma we can replace the sequence with convex combinations and get strong convergence and by going to a further subsequence we can assume that the limit is pointwise almost everywhere. As the functional is convex we still have a minimizing sequence. It follows from Fatou's Lemma that $(\tilde{\gamma},\tilde{\alpha}) \in \mathcal{M}_\kappa$. To show that $(\tilde{\gamma},\tilde{\alpha})$ is a minimizer we will prove that

$$\liminf_{n\to\infty}\mathcal{F}_\delta^{\text{aux}}(\gamma_n,\alpha_n) \ge \mathcal{F}_\delta^{\text{aux}}(\tilde{\gamma},\tilde{\alpha}).$$

Indeed,

$$\frac{1}{2}p^2\gamma_n(p) - Ts(\gamma_n(p),\alpha_n(p)) \ge \frac{1}{2}p^2\gamma_n(p) - Ts(\gamma_n(p),0) \ge T\ln(1-e^{-p^2/2T})$$

and the function on the right is integrable. Using the bound (4.6) we also see that $(\frac{1}{2}p^2-\delta)\gamma_n(p)$ is bounded below by an integrable function. The same is true for $\widehat{V}(p)(\gamma_n(p)+\alpha_n(p))$ using (3.5). The remaining quadratic terms have positive integrands. Hence the result follows by Fatou's Lemma. □

*Remark* 20. Lemma 18 implies that there exists a uniform bound on $\|\gamma_\kappa\|_1$. This follows from the obvious observation that $\hat{F}(\delta,\rho_0) \le 0$.

*Remark* 21. In one and two dimensions, the restriction defined in (4.6) has to be appropriately modified to obtain analogous results on the existence of minimizers for the restricted functional. In fact, one needs to assume

$\gamma(p) \leq \kappa/p^m$ with $m \in (\frac{1}{2}, 1)$ and $m \in (1,2)$ in one and two dimensions respectively.

One expects that by sending $\kappa \to \infty$ one approaches the minimizer of (4.3). In the next subsections we will implement this idea.

4.3. **A priori bounds on $\gamma$ and $\alpha$.** First, we show that any potential minimizer $\gamma$ is strictly positive almost everywhere.

**Lemma 22** (Positivity of $\gamma$)**.** *Suppose $(\gamma, \alpha)$ is a minimizer for either the unrestricted* (4.3) *or restricted* (4.5) *dual problem with $T > 0, \delta \in \mathbb{R}$, $\rho_0 \geq 0$, and $\kappa \geq T$. Then there exists a constant $C := C\left(\delta, \rho_0, \|\gamma\|_1, \widehat{V}\right)$ such that the set*

$$\mathcal{S} := \left\{ p \,|\, \gamma < e^{-\frac{p^2+C}{T}} \right\}.$$

*has zero measure.*

*Proof.* Since $\kappa \geq T$, we have $\kappa/p^2 \geq e^{-p^2/T}$ and the upper bound defining $\mathcal{S}$ is within the restriction in (4.6). The functional derivative [1] of $\mathcal{F}_\delta^{\text{aux}}$ in $\gamma$ gives

$$\frac{\partial \mathcal{F}_\delta^{\text{aux}}}{\partial \gamma} = p^2 - \delta + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma(p) - T \frac{\gamma + \frac{1}{2}}{\beta} \ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}.$$

Since $\frac{1}{2} \leq \beta = \sqrt{(\gamma + \frac{1}{2})^2 - \alpha^2} \leq \gamma + \frac{1}{2}$, we have

$$\frac{\partial \mathcal{F}_\delta^{\text{aux}}}{\partial \gamma} \leq p^2 + C - T \frac{\gamma + \frac{1}{2}}{\beta} \ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}} \leq p^2 + C - T \ln \frac{1}{\beta - \frac{1}{2}},$$

where $C := C\left(\delta, \rho_0, \|\gamma\|_1, \widehat{V}\right)$ follows from (3.6). Thus

$$\frac{\partial \mathcal{F}_\delta^{\text{aux}}}{\partial \gamma} < 0$$

if

$$\beta < e^{-\frac{p^2+C}{T}} + \frac{1}{2}.$$

Since $\beta \leq \gamma + \frac{1}{2}$, this certainly holds whenever

$$\gamma < e^{-\frac{p^2+C}{T}}.$$

Thus the functional derivative is negative for $p \in \mathcal{S}$. Hence, if the set had positive measure, we would be able to lower the free energy by increasing $\gamma$ on it. This would contradict the assumption that $(\gamma, \alpha)$ is a minimizer. $\square$

From now on we assume that $\kappa > T$. The next lemma provides a priori bounds on $\alpha$. We will show that $\alpha(p)^2 < \gamma(p)\left(\gamma(p) + 1\right)$ holds almost everywhere for minimizers of (4.3) or (4.5). Note that the statement is vacuous if $\gamma(p) = 0$. This possibility is, however, excluded (almost everywhere) by Lemma 22.

[1]We use the notation where $\frac{\partial \mathcal{F}_\delta^{\text{aux}}}{\partial \gamma}$ is defined by $\int \frac{\partial \mathcal{F}_\delta^{\text{aux}}}{\partial \gamma}(p)\phi(p)dp = \frac{d}{dt}\mathcal{F}_\delta^{\text{aux}}(\gamma + t\phi, \alpha)\big|_{t=0}$.

**Lemma 23.** *Suppose* $(\gamma, \alpha)$ *is a minimizer for either* (4.3) *or* (4.5) *with* $T > 0, \delta \in \mathbb{R}$ *and* $\rho_0 \geq 0$. *Then the set*

$$\mathcal{P} := \left\{ p \,|\, \alpha(p)^2 > \gamma(p)\left(\gamma(p)+1\right) - e^{-C/(Tc(\gamma(p)))},\ \alpha(p)^2 > \frac{1}{2}\gamma(p)\left(\gamma(p)+1\right) \right\}$$

*has zero measure. Here* $C := C\left(\rho_0, \|\gamma\|_1, \widehat{V}\right)$ *is a constant and*

$$c(\gamma) := \sqrt{\frac{2\gamma(\gamma+1)}{2\gamma(\gamma+1)+1}}.$$

*Proof.* The functional derivative of $\mathcal{F}_\delta^{\mathrm{aux}}$ in $\alpha$ gives

$$\frac{\partial \mathcal{F}_\delta^{\mathrm{aux}}}{\partial \alpha} = \rho_0 \widehat{V}(p) + \widehat{V} * \alpha(p) + T\frac{\alpha}{\beta}\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}}.$$

Assume first that $\alpha(p)^2 > \frac{1}{2}\gamma(p)\left(\gamma(p)+1\right)$. Then

$$\left|\frac{\alpha}{\beta}\right| \geq \sqrt{\frac{\frac{1}{2}\gamma\left(\gamma+1\right)}{\gamma(\gamma+1)+\frac{1}{4}-\alpha^2}} \geq \sqrt{\frac{\frac{1}{2}\gamma\left(\gamma+1\right)}{\frac{1}{2}\gamma(\gamma+1)+\frac{1}{4}}} = c(\gamma).$$

Another estimate that holds by the assumptions on $V$ and inequality (3.7) is

$$\left|\rho_0\widehat{V}(p) + \widehat{V} * \alpha(p)\right| \leq \rho_0\|\widehat{V}\|_\infty + \|\widehat{V} * \alpha\|_\infty \leq C\left(\rho_0, \|\gamma\|_1, \widehat{V}\right).$$

If $\alpha \geq \sqrt{\frac{1}{2}\gamma(p)(\gamma(p)+1)}$, then

$$\frac{\partial \mathcal{F}_\delta^{\mathrm{aux}}}{\partial \alpha} \geq -C + Tc(\gamma)\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}} \geq -C + Tc(\gamma)\ln\frac{1}{\beta-\frac{1}{2}},$$

where we have used $\beta \geq \frac{1}{2}$ in addition to the previous estimates. Similarly, if $\alpha \leq -\sqrt{\frac{1}{2}\gamma(p)(\gamma(p)+1)}$, we estimate

$$\frac{\partial \mathcal{F}_\delta^{\mathrm{aux}}}{\partial \alpha} \leq C - Tc(\gamma)\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}} \leq C - Tc(\gamma)\ln\frac{1}{\beta-\frac{1}{2}}.$$

In the first/second case the derivative is positive/negative whenever

$$\beta \leq \frac{1}{2} + e^{-C/(Tc(\gamma))},$$

and using the definition of $\beta^2$ we find that this happens when

$$\alpha^2 > \gamma(\gamma+1) - e^{-2C/(Tc(\gamma))} - e^{-C/(Tc(\gamma))}.$$

This means that the derivative is positive for $p$ in $\mathcal{P}$ and $\alpha(p) \geq 0$, and negative for $p$ in $\mathcal{P}$ and $\alpha(p) \leq 0$. Hence, if the set had positive measure, we would be able to lower the energy by varying on it, which contradicts the assumption that $(\gamma, \alpha)$ is a minimizer. □

Since we already know that $\gamma(p) > 0$ almost everywhere, this implies that $-\sqrt{\gamma(p)\left(\gamma(p)+1\right)} < \alpha(p) < \sqrt{\gamma(p)\left(\gamma(p)+1\right)}$ almost everywhere. Thus the Euler–Lagrange equation for $\alpha$ holds with equality for minimizers of both (4.3) and (4.5).

4.4. **A priori bound for $\gamma$ in the restricted case.** The existence of minimizers for (4.5), as well as the a priori bounds established in the previous subsection give us access to the Euler–Lagrange equations for the restricted problem. Indeed, we have

$$\begin{aligned}\frac{\partial \mathcal{F}^{\mathrm{aux}}_{\delta}}{\partial \gamma} &= p^2 - \delta + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma(p) - T\frac{\gamma+\frac{1}{2}}{\beta}\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}} \\ &= \begin{cases} \leq 0 & \text{if } \gamma(p) = \kappa/p^2 \\ = 0 & \text{if } 0 \leq \gamma(p) < \kappa/p^2 \end{cases} \end{aligned} \tag{4.8}$$

$$\frac{\partial \mathcal{F}^{\mathrm{aux}}_{\delta}}{\partial \alpha} = \rho_0 \widehat{V}(p) + \widehat{V} * \alpha(p) + T\frac{\alpha}{\beta}\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}} = 0. \tag{4.9}$$

We will now analyse these equations in order to derive a priori bounds for $\gamma_\kappa$, the minimizer of the restricted problem. These bounds will then be used to show convergence of $\gamma_\kappa$ to a minimizer of the unrestricted problem as $\kappa \to \infty$.

**Lemma 24** (Large $p$ a priori bound for $\gamma$)**.** *Let $T > 0$, $\delta \in \mathbb{R}$, and $0 \leq \rho_0 \leq \rho$. If $(\gamma, \alpha)$ is a minimizer for (4.5) with $\kappa > \max\{1, T\}$ there exist positive constants $P_0$ and $C$ such that for $|p| > P_0$, we have*

$$\gamma(p) \leq C|p|^{-4}. \tag{4.10}$$

*Moreover, as $T$ goes to zero $P_0$ is uniformly bounded below and $C$ uniformly bounded above.*

*Proof.* Assume $\alpha \neq 0$. Using (4.9), Lemma 18 and (3.7) we see that there is a $P_0$ such that for $|p| > P_0$

$$\begin{aligned} 0 \geq \frac{\partial \mathcal{F}^{\mathrm{aux}}_{\delta}}{\partial \gamma} &\geq \frac{1}{2}p^2 - T\frac{\gamma+\frac{1}{2}}{\beta}\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}} \\ &= \frac{1}{2}p^2 + \frac{\gamma+\frac{1}{2}}{\alpha}\Big(\rho_0\widehat{V}(p) + \widehat{V} * \alpha(p)\Big) \geq \frac{1}{2}p^2 - C\frac{\gamma+\frac{1}{2}}{|\alpha|}. \end{aligned} \tag{4.11}$$

Hence, we have

$$\frac{\alpha^2}{\left(\gamma+\frac{1}{2}\right)^2} \leq Cp^{-4}.$$

Note that we can now drop the assumption $\alpha \neq 0$ since the above also holds if $\alpha = 0$. This implies

$$\beta^2 = \left(\gamma + \frac{1}{2}\right)^2\left(1 - \frac{\alpha^2}{\left(\gamma+\frac{1}{2}\right)^2}\right) \geq \left(\gamma+\frac{1}{2}\right)^2\left(1 - Cp^{-4}\right),$$

which can be rewritten as

$$\frac{\gamma+\frac{1}{2}}{\beta} \leq \left(1 - Cp^{-4}\right)^{-\frac{1}{2}}. \tag{4.12}$$

Returning to the second estimate in (4.11), we obtain

$$0 \geq \frac{\partial \mathcal{F}^{\mathrm{aux}}_{\delta}}{\partial \gamma} \geq \frac{1}{2}p^2 - T\left(1 - Cp^{-4}\right)^{-\frac{1}{2}}\ln\frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}}.$$

Rewriting this inequality leads to

$$\beta \leq \frac{1}{2} \frac{\exp\left[\frac{p^2}{2T}\left(1-Cp^{-4}\right)^{1/2}\right]+1}{\exp\left[\frac{p^2}{2T}\left(1-Cp^{-4}\right)^{1/2}\right]-1} = \frac{1}{2} + \left[\exp\left[\frac{p^2}{2T}\left(1-Cp^{-4}\right)^{1/2}\right]-1\right]^{-1}.$$

Combining this with (4.12) we finally obtain

$$\gamma + \frac{1}{2} \leq \left(1-Cp^{-4}\right)^{-1/2}\left(\frac{1}{2} + \left[\exp\left[\frac{p^2}{2T}\left(1-Cp^{-4}\right)^{1/2}\right]-1\right]^{-1}\right),$$

which is $\frac{1}{2} + Cp^{-4} + \mathcal{O}(p^{-8})$ for $p$ large enough. □

Let $\gamma_\kappa$ be a minimizer for the restricted problem (4.5) for a given $\kappa$. We define

$$p_\kappa := \sup\left\{|p| \;\middle|\; \gamma_\kappa(p) = \frac{\kappa}{p^2}\right\}. \tag{4.13}$$

Note that the bound on $\gamma_\kappa$ for large $|p|$ proved in Lemma 24 implies that $p_\kappa$ cannot be infinite for any $\kappa$. We will therefore assume henceforth $p_\kappa$ is finite. It could be that $p_\kappa = -\infty$ (in case the set (4.13) is empty). In that case our proof works as well.

We shall now work towards a priori bounds on $\gamma$ for small $p$. We start by proving a lemma that we will use twice later on.

**Lemma 25.** *Let $a > 0$ and $f : [a,\infty) \to [0,\infty)$ be a non-negative, continuously differentiable function. If $|f'(t)| < C_a$ for $a \leq t \leq 2a$. Then*

$$\int_{|p|\geq a} f(|p|)^{-1} d^3p \geq (2\pi^2)^{-1} a^2 {C_a}^{-1} \ln\left(1 + \frac{C_a}{f(a)} a\right).$$

*Proof.* By assumption we have $f(|p|) \leq f(a) + C_a(|p| - a)$ for $a \leq |p| \leq 2a$. Thus (recalling our convention for the measures $dp$ and $dt$ explained above (4.1))

$$\begin{aligned}\int_{|p|\geq a} f(|p|)^{-1} d^3p &\geq (2\pi^2)^{-1} \int_a^{2a} \left[f(a) + C_a(t-a)\right]^{-1} t^2 dt \\ &\geq (2\pi^2)^{-1} a^2 \int_0^a \left[f(a) + C_a t\right]^{-1} dt \\ &= (2\pi^2)^{-1} a^2 {C_a}^{-1} \ln\left(1 + \frac{C_a}{f(a)} a\right).\end{aligned}$$

□

To obtain the desired bound for small $p$ we will apply this lemma to the radial function $\tilde{f}$ given by

$$\tilde{f}(|p|) := \gamma_\kappa(p)^{-1}, \tag{4.14}$$

where $\gamma_\kappa$ is a minimizer for the restricted problem (note this is indeed a radial function by Lemma 17).

To this end we need to get a bound on the derivative of $\gamma_\kappa^{-1}$. In the calculations below we assume $(\gamma, \alpha)$ is a minimizer for (4.5) for a fixed $\delta \in \mathbb{R}$ and $\rho_0 \geq 0$ (we drop the subscript $\kappa$ for convenience).

We start our analysis from the Euler–Lagrange equations, which hold with equality for $|p| > p_\kappa$ :

$$\begin{aligned} \frac{\partial \mathcal{F}^{\text{aux}}_\delta}{\partial \gamma} &= p^2 - \delta + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma(p) - T\frac{\gamma + \frac{1}{2}}{\beta} \ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}} = 0 \\ \frac{\partial \mathcal{F}^{\text{aux}}_\delta}{\partial \alpha} &= \rho_0 \widehat{V}(p) + \widehat{V} * \alpha(p) + T\frac{\alpha}{\beta} \ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}} = 0. \end{aligned} \tag{4.15}$$

By squaring, subtracting and taking a square root we obtain

$$\ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}} = \frac{1}{T}\sqrt{\left(p^2 - \delta + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma(p)\right)^2 - \left(\rho_0 \widehat{V}(p) + \widehat{V} * \alpha(p)\right)^2},$$

which we denote by $G(p)$. In particular, we have

$$\beta = \frac{1}{2}\frac{e^G + 1}{e^G - 1}.$$

We also define

$$\begin{aligned} A(p) &:= \frac{1}{T}\left(p^2 - \delta + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma(p)\right) \\ B(p) &:= \frac{1}{T}\left(\rho_0 \widehat{V}(p) + \widehat{V} * \alpha(p)\right). \end{aligned} \tag{4.16}$$

Combined with (4.15) this leads to

$$\gamma = \beta \left[\ln \frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}\right]^{-1} A - \frac{1}{2} = \frac{1}{2}\left[\frac{e^G + 1}{G(e^G - 1)}A - 1\right]. \tag{4.17}$$

We know that $\gamma \le \kappa/p^2$ and also that the expression above is correct for $|p| > p_\kappa$. Therefore the denominator cannot go to zero in this region (implying $G$ cannot go to zero). Combining this with the relation between $G$ and $A$ we obtain

$$A \ge G > 0. \tag{4.18}$$

Together with (4.17), this implies

$$\gamma^{-1} = \frac{2G(e^G - 1)}{e^G(A - G) + A + G} \le (e^G - 1) \le (e^A - 1). \tag{4.19}$$

Recall the definition (4.14). From (4.19) it follows that on $(p_k, \infty)$ we have

$$\begin{aligned} \frac{\tilde{f}'(|p|)}{2} =& \frac{G'\left[e^G - 1 + Ge^G\right]}{D} \\ &- \frac{G(e^G - 1)\left[G'e^G(A - G) + A'(e^G + 1) + G'(1 - e^G)\right]}{D^2} \\ =& \frac{1}{D}\left[GG'\left(\frac{e^G - 1}{G} + e^G\right)\right] - GG'\frac{G}{D}\frac{e^G - 1}{G}e^G\left[\frac{A}{D} - \frac{G}{D}\right] \\ &- A'\left(\frac{G}{D}\right)^2\frac{e^G - 1}{G}\left(e^G + 1\right) + GG'\left(\frac{e^G - 1}{G}\right)^2\left(\frac{G}{D}\right)^2, \end{aligned}$$

where $D = e^G(A - G) + A + G$. Note that if $P > p_\kappa$ is bounded then all terms except the first are bounded on $p_k < |p| \le P$: $A$ and $A'$ are bounded by their form (4.16) and the assumptions on $V$; $G$ is bounded by $A$; $D$ is bigger than or equal to both $G$ and $A$. The boundedness of $GG'$ follows from

$$G' = \frac{1}{G}\left(AA' + BB'\right)$$

and the boundedness from all terms between the brackets ($B$ and $B'$ are bounded for similar reasons as $A$ and $A'$). It follows that

$$\tilde{f}'(p) \leq \frac{C_2}{D(p)} + C_3 \leq \frac{C_2}{A(p)} + C_3,$$

where the $C_i := C_i(P, \|\widehat{V}\|_\infty, \|\nabla\widehat{V}\|_\infty, \|\gamma\|_1)$ are constants. To obtain a final bound on $\tilde{f}'(p)$ we need the following lemma.

**Lemma 26.** *For $p_\kappa < |p| \leq \frac{1}{2}P$, where $P > 2p_\kappa$ is a given constant, we have*

$$A(p) \geq \ln\left[1 + C_1|p|e^{-\frac{2\pi^2 C_1\|\gamma\|_1}{p^2}}\right],$$

*where $C_1 := C_1(P, \|\widehat{V}\|_\infty, \|\nabla\widehat{V}\|_\infty, \|\gamma\|_1)$ is a constant.*

*Proof.* In order to apply Lemma 25 we define the function

$$f(|p|) := e^{A(p)} - 1.$$

By (4.16), (4.18) and our assumptions on $V$ it follows that $f$ is positive and continuously differentiable. To apply Lemma 25, we need a bound on its derivative for $|p| \in (p_\kappa, P)$. Since $A$ and $A'$ are bounded for $p_\kappa < |p| \leq P$ we have

$$|f'(|p|)| = |A'(|p|)|e^{A(|p|)} \leq C_1(P, \|\widehat{V}\|_\infty, \|\nabla\widehat{V}\|_\infty, \|\gamma\|_1).$$

Using Lemma 25 and (4.19), we now get for $p_\kappa < |p| \leq \frac{1}{2}P$

$$\|\gamma\|_1 \geq \int_{|\xi|\geq|p|} f(|\xi|)^{-1} d^3\xi \geq (2\pi^2)^{-1}p^2 C_1^{-1} \ln\left[1 + C_1|p|(e^{A(p)} - 1)^{-1}\right].$$

Rewriting this proves the lemma. □

It follows that

$$\tilde{f}'(p) \leq \frac{C_2}{\ln\left[1 + C_1|p|e^{-\frac{2\pi^2 C_1\|\gamma\|_1}{p^2}}\right]} + C_3 =: \eta(|p|). \tag{4.20}$$

Since the function $\eta$ is decreasing, we can bound it on the interval $[|p|, 2|p|]$ by its value at $|p|$.

**Lemma 27** (Small $p$ a priori bound for $\gamma$)**.** *For $p_k < |p| \leq P_0$ (where $P_0$ was defined in Lemma 24), we have*

$$\gamma(p) \leq |p|^{-1}\eta(|p|)^{-1}e^{\frac{2\pi^2\|\gamma\|_1\eta(|p|)}{p^2}}, \tag{4.21}$$

*where $\eta$ is defined in (4.20) with $P$ replaced by $2P_0$ (in the dependence of the constants).*

*Proof.* Equation (4.20) gives us the bound required to apply Lemma 25. We therefore get

$$\|\gamma\|_1 \geq \int_{|\xi|\geq|p|} \tilde{f}(|\xi|)^{-1} d^3\xi \geq (2\pi^2)^{-1} p^2 \eta(|p|)^{-1} \ln\left[1 + |p|\eta(|p|)\gamma(p)\right],$$

which gives the stated result upon rewriting. □

*Remark* 28. All a priori bounds derived in this subsection remain (up to minor modifications) true in one and two dimensions.

Equipped with these bounds we shall move towards the proof of existence of minimizer for the dual auxiliary problem.

4.5. **Existence of minimizers for the dual auxiliary problem.** In this section we prove the existence of a minimizer for $F^{\text{aux}}(\lambda^{\min}, \rho_0^{\min})$, where $(\lambda^{\min}, \rho_0^{\min})$ corresponds to the minimum of the function $F^{\text{aux}}(\lambda, \rho_0)$. As explained before, this is equivalent to finding a minimizer for $\hat{F}^{\text{aux}}(\delta^{\min}, \rho_0^{\min})$ (recall (4.1) and (4.3)), and therefore, by Proposition 14, to the existence of minimizers for the initial problems (1.2) and (1.4). The goal of this subsection is thus to prove the following theorem.

**Theorem 29** (Existence of unconstrained minimizers)**.** *There exists a minimizer* $(\tilde{\gamma}, \tilde{\alpha})$ *for the dual auxiliary problem* (4.3) *with* $\delta = \delta^{\min}$, $\rho_0 = \rho_0^{\min}$ *and* $T > 0$.

As we have proved in Proposition 19, for given $\delta$, $\rho_0$ and $\kappa$ we can find $(\gamma_\kappa, \alpha_\kappa)$ that minimize the restricted problem (4.5). We would like to combine the bounds in Lemmas 24 and 27 to extract a minimizer for the dual auxiliary problem (4.3) from the sequence $(\gamma_\kappa, \alpha_\kappa)$. To do this, we first need to prove that we can actually reach the whole of $|p| > 0$ using the regions $|p| > p_\kappa$.

**Lemma 30.** *There exists a subsequence of* $(\gamma_\kappa, \alpha_\kappa)$ *such that* $p_\kappa \to 0$ *as* $\kappa \to \infty$.

*Proof.* First note that the assumption that $\liminf_{\kappa\to\infty} p_\kappa = c > 0$ together with Lemma 27 and the uniform bound on $\|\gamma_\kappa\|_1$ will lead to a contradiction if we can show that

$$\lim_{|p|\searrow p_\kappa} \gamma_k(p) = \frac{\kappa}{p_\kappa^2}. \tag{4.22}$$

Indeed, in this situation the left-hand side of (4.21) tends to infinity, whereas the right-hand side is bounded yielding a contradiction. We conclude that $\liminf_{\kappa\to\infty} p_\kappa \leq 0$ and hence we can extract a subsequence that has $p_\kappa \to 0$.

To prove (4.22), we first claim there exist $\tilde{\gamma}, \tilde{\alpha}$ and associated $\tilde{\beta}$ such that

$$\begin{aligned} p^2 - \delta + \rho_0\widehat{V}(p) + \widehat{V} * \gamma_\kappa(p) - T\frac{\tilde{\gamma}+\frac{1}{2}}{\tilde{\beta}} \ln\frac{\tilde{\beta}+\frac{1}{2}}{\tilde{\beta}-\frac{1}{2}} &= 0 \\ \rho_0\widehat{V}(p) + \widehat{V} * \alpha_\kappa(p) + T\frac{\tilde{\alpha}}{\tilde{\beta}} \ln\frac{\tilde{\beta}+\frac{1}{2}}{\tilde{\beta}-\frac{1}{2}} &= 0 \end{aligned} \tag{4.23}$$

is satisfied for $|p| > p_\kappa - \varepsilon$ for some $\varepsilon > 0$. Of course we know that $(\gamma_\kappa, \alpha_\kappa)$ fulfils this equation for $|p| > p_\kappa$, but we can do a little better. To see that such $\tilde{\gamma}$ and $\tilde{\alpha}$ exist, consider the explicit expression (4.17) for $\tilde{\gamma}$ in terms of

$G$ and $A$ which follows from (4.23) as before (and only depends on $\gamma_\kappa$ and $\alpha_\kappa$). In particular, we know that as long as $|p| \geq p_\kappa$ the denominator in (4.17) does not go to zero since the $\gamma_\kappa \leq \kappa/p^2$ for $|p| > p_\kappa$. Since $G$ and $A$ are continuous everywhere, we can infer that there has to be a small region $|p| > p_\kappa - \varepsilon$ where there exist continuous $\tilde{\gamma}$ and $\tilde{\alpha}$ that satisfy (4.23) (which have to coincide with $\gamma_\kappa$ for $|p| > p_\kappa$, but may not do so otherwise).

Now suppose that $\tilde{\gamma}(p) < \kappa/p_\kappa^2$ for $|p| = p_\kappa$. By continuity and the argument above, we then also have that $\tilde{\gamma}(p) < \kappa/p^2$ on (a possibly smaller region) $p_\kappa - \varepsilon < |p| \leq p_\kappa$. By the definition of $p_\kappa$ we must then have that $\gamma_\kappa(p) > \tilde{\gamma}(p)$ on a set of positive measure. Since the entropy derivative is strictly increasing in $\gamma$, we have for such $p$ that

$$\frac{\partial \mathcal{F}_\delta^{\text{aux}}}{\partial \gamma_\kappa} = p^2 - \delta + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma_\kappa(p) - T\frac{\gamma_\kappa + \frac{1}{2}}{\beta_k} \ln \frac{\beta_k + \frac{1}{2}}{\beta_k - \frac{1}{2}} > 0.$$

This contradicts the fact that $\gamma_\kappa$ is part of a minimizer (which should always satisfy (4.8)). We conclude that (4.22) is true. □

This lemma implies that we can pick a subsequence $p_\kappa$ that is decreasing and tends to zero. This is what we will assume from now on.

We now show that the corresponding $(\gamma_\kappa, \alpha_\kappa)$ form a minimizing sequence of the dual auxiliary problem (4.3).

**Lemma 31.** *Let* $(\gamma_k, \alpha_k, \rho_0)$ *be minimizers for the restricted problem* (4.5)*. We then have*

$$\lim_{\kappa\to\infty} \mathcal{F}_\delta^{\text{aux}}(\gamma_\kappa, \alpha_\kappa, \rho_0) = \inf_{(\gamma,\alpha)\in\mathcal{D}'} \mathcal{F}_\delta^{\text{aux}}(\gamma, \alpha, \rho_0).$$

*Proof.* Let $(\gamma, \alpha)$ be a general element in $\mathcal{D}'$. We will show that its energy can always be approximated by the energy of a sequence of elements in $\mathcal{M}_\kappa$. We simply define the functions:

$$\tilde{\gamma}_\kappa = \gamma \; \mathbb{1}(\gamma \leq \kappa/p^2)$$
$$\tilde{\alpha}_\kappa = \alpha \; \mathbb{1}(\gamma \leq \kappa/p^2),$$

which implies $(\tilde{\gamma}_\kappa, \tilde{\alpha}_\kappa) \in \mathcal{M}_\kappa$. It follows from Lebesgue's Dominated Convergence Theorem that

$$\mathcal{F}_\delta^{\text{aux}}(\tilde{\gamma}_\kappa, \tilde{\alpha}_\kappa, \rho_0) \to \mathcal{F}_\delta^{\text{aux}}(\gamma, \alpha, \rho_0).$$

Since we know that the $(\gamma_\kappa, \alpha_\kappa)$ are minimizers for the restricted problems, we have

$$\mathcal{F}_\delta^{\text{aux}}(\gamma_\kappa, \alpha_\kappa, \rho_0) \leq \mathcal{F}_\delta^{\text{aux}}(\tilde{\gamma}_\kappa, \tilde{\alpha}_\kappa, \rho_0).$$

By taking a limit in $\kappa$ followed by an infimum over $\mathcal{D}'$, we obtain

$$\limsup_{\kappa\to\infty} \mathcal{F}_\delta^{\text{aux}}(\gamma_\kappa, \alpha_\kappa, \rho_0) \leq \inf_{\mathcal{D}'} \mathcal{F}_\delta^{\text{aux}}(\gamma, \alpha, \rho_0),$$

which in combination with the easy observation (use $\mathcal{M}_\kappa \subset \mathcal{D}'$ to get the inequality and then take the lim inf)

$$\inf_{\mathcal{D}'} \mathcal{F}_\delta^{\text{aux}}(\gamma, \alpha, \rho_0) \leq \liminf_{\kappa\to\infty} \mathcal{F}_\delta^{\text{aux}}(\gamma_\kappa, \alpha_\kappa, \rho_0)$$

leads to the desired conclusion. □

We will now construct a candidate minimizer $(\tilde{\gamma}, \tilde{\alpha})$ from the restricted minimizers $(\gamma_\kappa, \alpha_\kappa)$. Now it will be important that we are dealing with $(\delta^{\min}, \rho_0^{\min})$ and not just any $(\delta, \rho_0)$.

**Proposition 32.** *Let $(\gamma_\kappa, \alpha_\kappa)$ be a sequence of minimizers for $\hat{F}_\kappa^{\text{aux}}(\delta^{\min}, \rho_0^{\min})$ (and hence a minimizing sequence for the dual auxiliary problem), such that $p_\kappa$ decreases to zero. We can extract a new minimizing sequence, denoted also $(\gamma_\kappa, \alpha_\kappa)$, such that $\gamma_\kappa \to \tilde{\gamma}$ pointwise and in $L^1$, and $\alpha_\kappa \to \tilde{\alpha}$ pointwise and $(\tilde{\gamma}, \tilde{\alpha}) \in \mathcal{D}'$.*

*Proof. Step 1. - pointwise convergence.* Recall definition (4.13). For a given $p \in \mathbb{R}^3$ define $\kappa_0(p)$ to be the smallest $\kappa$ such that $p_\kappa < |p|$. Let $h(p) := \kappa_0(p)/p^2$. Let us call $l(p)$ the function that defines the a priori large $p$ upper bound on $\gamma(p)$, i.e. $l(p)$ is the RHS of (4.10). Similarly, let $s(p)$ be the function that defines the a priori small $p$ upper bound on $\gamma(p)$, i.e. $s(p)$ is the RHS of (4.21). Note that using the fact that $\|\gamma_\kappa\|_1$ is bounded uniformly in $\kappa$, the bound $s(p)$ can be modified to be $\kappa$-independent. We call this new bound $s(p)$ as well. We then define the function

$$K(p) = \max\{h(p), l(p), s(p)\}.$$

Note that for any $\kappa$ we have

$$\gamma_\kappa(p) \leq K(p).$$

Indeed, given a $\gamma_\kappa$ and $p$ we either have $\kappa \leq \kappa_0(p)$ or $\kappa > \kappa_0(p)$. In the first case we clearly have $\gamma_\kappa(p) \leq \kappa/p^2 \leq h(p)$. In the second case, by definition, we have $p_\kappa \leq |p|$ and thus $\gamma_\kappa(p) \leq \max\{l(p), s(p)\}$.

We use the function $K(p)$ to introduce the weighted $L^2$-space with the measure $d\mu(p) = \frac{f(p)dp}{(K(p))^2}$ where $f(p)$ is a strictly positive $L^1$-function such that the measure is finite ($f$ has to decay sufficiently fast). We then have the uniform bounds

$$\|\gamma_\kappa\|^2_{L^2(d\mu(p))} = \int \frac{\gamma_\kappa^2 f}{K^2} \leq \int f < C,$$
$$\|\alpha_\kappa\|^2_{L^2(d\mu(p))} = \int \frac{\alpha_\kappa^2 f}{K^2} \leq \int \frac{(\gamma_\kappa^2 + \gamma_\kappa) f}{K^2} \leq C + \frac{1}{2}\int \frac{\gamma_\kappa^2 f}{K^2} + \frac{1}{2}\int \frac{f}{K^2} < C.$$

These bounds allow us to extract a subsequence $(\gamma_\kappa, \alpha_\kappa)$ that converges weakly in the weighted $L^2$-space. Next, applying Mazur's Lemma, we can obtain a strongly converging sequence of convex combinations, which – by convexity of the functional (recall Lemma 15) – is also a minimizing sequence. Picking a further subsequence we can obtain a pointwise converging subsequence. We denote the limiting functions by $\tilde{\gamma}$ and $\tilde{\alpha}$. By the pointwise convergence we have $\tilde{\alpha}^2 \leq \tilde{\gamma}(\tilde{\gamma} + 1)$.

*Step 2.* Fatou's lemma in combination with pointwise convergence implies that

$$\int (1+p^2)\tilde{\gamma} = \int \liminf_{\kappa\to\infty} (1+p^2)\gamma_\kappa \leq \liminf_{\kappa\to\infty} \int (1+p^2)\gamma_\kappa. \tag{4.24}$$

Recall that we have a uniform bound on $\|\gamma_\kappa\|_{L^1((1+p^2)dp)}$. This means that the integral on the left-hand side is bounded and therefore $\tilde{\gamma} \in L^1((1+p^2)dp)$.

*Step 3 - $L^1$-convergence.* By Lemma 31 we know that $(\gamma_\kappa, \alpha_\kappa)$ form a minimizing sequence. Thus, as we consider $\delta^{\min}$, it follows that $\int \gamma_\kappa \to \lambda^{\min}$.

Recall that the $\gamma_\kappa$ are uniformly bounded by an $L^1$ function on intervals $[\varepsilon, \infty)$. This implies

$$\int_{|p|>\varepsilon} \gamma_\kappa \xrightarrow{\kappa\to\infty} \int_{|p|>\varepsilon} \tilde{\gamma} \xrightarrow{\varepsilon\to 0} \int \tilde{\gamma} \tag{4.25}$$

where the first convergence follows by an application of the Dominated Convergence Theorem (we have pointwise convergence and a uniform $L^1$-bound by (4.10) and (4.21)), and the second by the Monotone Convergence Theorem. Furthermore, it follows from Fatou's lemma that $\int \tilde{\gamma} \leq \lambda^{\min}$. First that $\int \tilde{\gamma} = \lambda^{\min}$. We use this to see that

$$\begin{aligned}\int |\tilde{\gamma} - \gamma_\kappa| &\leq \int_{|p|>\varepsilon} |\tilde{\gamma} - \gamma_\kappa| + \int_{|p|\leq\varepsilon} \tilde{\gamma} + \int_{|p|\leq\varepsilon} \gamma_\kappa \\ &\leq \int_{|p|>\varepsilon} |\tilde{\gamma} - \gamma_\kappa| + \int_{|p|\leq\varepsilon} \tilde{\gamma} + \int \gamma_\kappa - \int_{|p|>\varepsilon} \gamma_\kappa.\end{aligned}$$

We use our observation (4.25) for the fourth term and apply the Dominated Convergence Theorem to the first term to obtain

$$\limsup_{\kappa\to\infty} \int |\tilde{\gamma} - \gamma_\kappa| \leq \int_{|p|\leq\varepsilon} \tilde{\gamma} + \lambda^{\min} - \int_{|p|>\varepsilon} \tilde{\gamma} \xrightarrow{\varepsilon\to 0} 0.$$

Here, the last terms cancel because of our assumption on $\int \tilde{\gamma}$ and the convergence in $\varepsilon$ holds simply because $\tilde{\gamma} \in L^1$. This means that in this case we have proved the proposition. It remains to show that $\int \tilde{\gamma} < \lambda^{\min}$ is impossible.

*Step 4.* Assume $\int \tilde{\gamma} < \lambda^{\min}$. We have

$$\int_{|p|\leq\varepsilon} \gamma_\kappa = \int \gamma_\kappa - \int_{|p|>\varepsilon} \gamma_\kappa \xrightarrow{\kappa\to\infty} \lambda^{\min} - \int_{|p|>\varepsilon} \tilde{\gamma} \xrightarrow{\varepsilon\to 0} \lambda^{\min} - \int \tilde{\gamma} > 0.$$

This quantity is important for our proof, so we give it a name:

$$d := \lim_{\varepsilon\to 0} \lim_{\kappa\to\infty} \int_{|p|\leq\varepsilon} \gamma_\kappa > 0.$$

We start with the following estimate (throwing out some positive terms, using (3.5) and estimating the entropy for small $p$):

$$
\begin{aligned}
\mathcal{F}^{\text{aux}}(\gamma_\kappa,\alpha_\kappa,\rho_0^{\min}) \geq & \int_{|p|>\varepsilon} p^2\gamma_\kappa + \rho_0^{\min}\int_{|p|>\varepsilon}\widehat{V}(\gamma_\kappa+\alpha_\kappa) - \frac{1}{2}\rho_0^{\min}\int_{|p|\leq\varepsilon}\widehat{V} \\
& - T\int_{|p|>\varepsilon} s(\gamma_\kappa,\alpha_\kappa) - CT\varepsilon^3 - CT\|\gamma_\kappa\|_1^{\frac{1}{2}}\varepsilon^{3/2} \\
& + \frac{1}{2}\int_{|p|>\varepsilon}\int_{|q|>\varepsilon}\widehat{V}(p-q)(\gamma_\kappa(p)\gamma_\kappa(q)+\alpha_\kappa(p)\alpha_\kappa(q))dqdp \\
& + \int_{|p|\leq\varepsilon}\int_{|q|>\varepsilon}\widehat{V}(q-p)(\gamma_\kappa(p)\gamma_\kappa(q)+\alpha_\kappa(p)\alpha_\kappa(q))dqdp \\
& + \frac{1}{2}\int_{|p|\leq\varepsilon}\int_{|q|\leq\varepsilon}\widehat{V}(p-q)\gamma_\kappa(p)\gamma_\kappa(q)dqdp.
\end{aligned}
\tag{4.26}
$$

Note that we have obtained the term in the fourth line twice since $\widehat{V}$ is radial, which implies $\widehat{V}(p-q)=\widehat{V}(q-p)$. For the entropy, we have used

$$
\int_{|p|<\varepsilon} s(\gamma,\alpha) \leq \int_{|p|<\varepsilon} s(\gamma,0) = \int_{|p|<\varepsilon}(1+\gamma)\ln(1+\gamma)-\gamma\ln\gamma. \tag{4.27}
$$

In the region where $\gamma\leq 1$, the integrand is bounded by $2\ln(2)+1$. In the region where $\gamma>1$, we have

$$
(1+\gamma)\ln(1+\gamma)-\gamma\ln\gamma = \ln\gamma+(1+\gamma)\ln(1+\gamma^{-1}) \leq \ln\gamma+1+\gamma^{-1} \leq \sqrt{\gamma}+2.
$$

Together with (4.27), using Cauchy–Schwarz, this implies that

$$
\int_{|p|<\varepsilon} s(\gamma,\alpha) \leq C\varepsilon^3 + C\|\gamma_\kappa\|_1^{\frac{1}{2}}\varepsilon^{3/2}.
$$

Continuing from (4.26), for $|p|\leq\varepsilon$ we estimate

$$
\left|\int_{|q|>\varepsilon}\widehat{V}(q)\gamma_\kappa(q)dq - \int_{|q|>\varepsilon}\widehat{V}(q-p)\gamma_\kappa(q)dq\right| \leq \varepsilon\|\nabla\widehat{V}\|_\infty\|\gamma_\kappa\|_1, \tag{4.28}
$$

where we have used our assumptions on the differentiability of $\widehat{V}$. To see that a similar estimate holds for $\alpha_\kappa$, we note that by an argument identical to (3.7) we have

$$
\left\|\nabla\int_{|q|>\varepsilon}\widehat{V}(q-p)\alpha_\kappa(q)dq\right\|_\infty = \left\|\int_{|q|>\varepsilon}\nabla\widehat{V}(q-p)\alpha_\kappa(q)dq\right\|_\infty \leq C
$$

where $C$ is a constant that can be chosen independent of $\kappa$. For $|p|\leq\varepsilon$ this leads to

$$
\left|\int_{|q|>\varepsilon}\widehat{V}(q)\alpha_\kappa(q) - \int_{|q|>\varepsilon}\widehat{V}(q-p)\alpha_\kappa(q)\right| \leq \varepsilon C.
$$

Finally, for $|q|\leq\varepsilon$,

$$
\left|\int_{|p|\leq\varepsilon}\widehat{V}(0)\gamma_\kappa(p) - \int_{|p|\leq\varepsilon}\widehat{V}(p-q)\gamma_\kappa(p)\right| \leq 2\varepsilon\|\nabla\widehat{V}\|_\infty\|\gamma_\kappa\|_1.
$$

Using the last two estimates together with (4.28) in (4.26) and estimating the third term of (4.26), we obtain

$$
\begin{aligned}
\mathcal{F}^{\rm aux}(\gamma_\kappa,\alpha_\kappa,\rho_0^{\rm min}) \geq & \int_{|p|>\varepsilon} p^2\gamma_\kappa + \rho_0^{\rm min}\int_{|p|>\varepsilon}\widehat{V}(\gamma_\kappa+\alpha_\kappa) - T\int_{|p|>\varepsilon} s(\gamma_\kappa,\alpha_\kappa) \\
& + \frac{1}{2}\int_{|p|>\varepsilon}\int_{|q|>\varepsilon}\widehat{V}(p-q)(\gamma_\kappa(p)\gamma_\kappa(q)+\alpha_\kappa(p)\alpha_\kappa(q))dqdp \\
& + \left(\int_{|p|\leq\varepsilon}\gamma_\kappa(p)dp\right)\left[\int_{|q|>\varepsilon}\widehat{V}(q)\gamma_\kappa(q)dq - \varepsilon\|\nabla\widehat{V}\|_\infty\|\gamma_\kappa\|_1\right] \\
& - \left|\int_{|p|\leq\varepsilon}\alpha_\kappa(p)dp\right|\left[\left|\int_{|q|>\varepsilon}\widehat{V}(q)\alpha_\kappa(q)dq\right| + \varepsilon C\left(\|\gamma_\kappa\|_1,\nabla\widehat{V}\right)\right] \\
& + \frac{1}{2}\left(\int_{|q|\leq\varepsilon}\gamma_\kappa(p)dp\right)\left[\widehat{V}(0)\int_{|p|\leq\varepsilon}\gamma_\kappa(q)dq - 2\varepsilon\|\nabla\widehat{V}\|_\infty\|\gamma_\kappa\|_1\right] \\
& - C\rho_0^{\rm min}\|\widehat{V}\|_\infty - CT\varepsilon^3 - CT\|\gamma_\kappa\|_1^{\frac{1}{2}}\varepsilon^{3/2}.
\end{aligned}
$$

Since $|\alpha_\kappa| \leq \gamma_\kappa + 1/2$, we see that

$$
\left|\int_{|p|\leq\varepsilon}\alpha_\kappa(p)dp\right| \leq \int_{|p|\leq\varepsilon}\gamma_\kappa(p)dp + C\varepsilon^3. \tag{4.29}
$$

and hence all the error terms in this expression tend to zero as $\varepsilon\to 0$.

We now choose $\kappa(\varepsilon)$ such that it tends to infinity as $\varepsilon\to 0$ and such that $\left|\lim_{\kappa\to\infty}\int_{|p|<\varepsilon}\gamma_\kappa - \int_{|p|<\varepsilon}\gamma_{\kappa(\varepsilon)}\right| < \varepsilon$. Then, in particular,

$$
\lim_{\varepsilon\to 0}\int_{|p|<\varepsilon}\gamma_{\kappa(\varepsilon)} - d \to 0. \tag{4.30}
$$

Combining this with (4.29) we find that

$$
\begin{aligned}
& \mathcal{F}^{\rm aux}(\gamma_{\kappa(\varepsilon)},\alpha_{\kappa(\varepsilon)},\rho_0^{\rm min}) \\
& \geq \int_{|p|>\varepsilon} p^2\gamma_{\kappa(\varepsilon)} - T\int_{|p|>\varepsilon} s(\gamma_{\kappa(\varepsilon)},\alpha_{\kappa(\varepsilon)}) \\
& \quad +\rho_0^{\rm min}\left(\int_{|p|>\varepsilon}\widehat{V}\gamma_{\kappa(\varepsilon)} - \left|\int_{|p|>\varepsilon}\widehat{V}\alpha_{\kappa(\varepsilon)}\right|\right) \\
& \quad +\frac{1}{2}\int_{|p|>\varepsilon}\int_{|q|>\varepsilon}\widehat{V}(p-q)(\gamma_{\kappa(\varepsilon)}(p)\gamma_{\kappa(\varepsilon)}(q)+\alpha_{\kappa(\varepsilon)}(p)\alpha_{\kappa(\varepsilon)}(q))dqdp \\
& \quad +d\int_{|p|>\varepsilon}\widehat{V}\gamma_{\kappa(\varepsilon)} - d\left|\int_{|p|>\varepsilon}\widehat{V}\alpha_{\kappa(\varepsilon)}\right| + \frac{1}{2}d^2\widehat{V}(0) - c(\varepsilon),
\end{aligned}
$$

where the error $c(\varepsilon)$ tends to zero as $\varepsilon\to 0$. We now define

$$
\begin{aligned}
\tilde{\gamma}_\varepsilon &= \gamma_{\kappa(\varepsilon)}\ \mathbb{1}(|p|>\varepsilon) \\
\tilde{\alpha}_\varepsilon &= \pm\alpha_{\kappa(\varepsilon)}\ \mathbb{1}(|p|>\varepsilon),
\end{aligned}
$$

where the sign $\pm$ in the second equation is chosen such that

$$
\int_{|p|\geq\varepsilon}\widehat{V}\tilde{\alpha}_\varepsilon \leq 0.
$$

Then

$$\mathcal{F}^{\text{aux}}(\gamma_{\kappa(\varepsilon)}, \alpha_{\kappa(\varepsilon)}, \rho_0^{\min}) \geq \mathcal{F}^{\text{aux}}(\tilde{\gamma}_\varepsilon, \tilde{\alpha}_\varepsilon, \rho_0^{\min} + d) + \frac{1}{2}d^2\widehat{V}(0) - c(\varepsilon). \quad (4.31)$$

We will now show how (4.31) leads to a contradiction if $d > 0$. We first use that applying the Legendre transform twice on a convex function yields the original function (recall that $F^{\text{aux}}(\lambda, \rho_0)$ is convex in $\lambda$). Thus

$$F^{\text{aux}}(\lambda, \rho_0) = \sup_\delta \left[ \inf_{\lambda'} \left[ F^{\text{aux}}(\lambda', \rho_0) - \delta\lambda' \right] + \delta\lambda \right],$$

and hence

$$F^{\text{aux}}(\lambda, \rho_0) = \sup_\delta \left[ \inf_{(\gamma,\alpha)\in\mathcal{D}'} \left[ \mathcal{F}^{\text{aux}}(\gamma, \alpha, \rho_0) - \delta \int \gamma \right] + \delta\lambda \right]. \quad (4.32)$$

Using Lemma 31 (recall that $\mathcal{F}^{\text{aux}}_\delta(\gamma, \alpha, \rho_0) = \mathcal{F}^{\text{aux}}(\gamma, \alpha, \rho_0) - \delta \int \gamma$) we note that for any $\delta \in \mathbb{R}$:

$$F^{\text{aux}}(\lambda^{\min}, \rho_0^{\min}) \geq \lim_{\kappa\to\infty} \left[ \mathcal{F}^{\text{aux}}(\gamma_\kappa, \alpha_\kappa, \rho_0^{\min}) - \delta \int \gamma_\kappa \right] + \delta\lambda^{\min}.$$

Recalling our conclusion (4.31) and that (4.30) gives $\lim_{\varepsilon\to 0} \int (\gamma_{\kappa(\varepsilon)} - \tilde{\gamma}_\varepsilon) = d$, we obtain

$$\begin{aligned} F^{\text{aux}}(\lambda^{\min}, \rho_0^{\min}) &\geq \liminf_{\varepsilon\to 0} \left[ \mathcal{F}^{\text{aux}}(\tilde{\gamma}_\varepsilon, \tilde{\alpha}_\varepsilon, \rho_0^{\min} + d) - \delta \left( \int \tilde{\gamma}_\varepsilon + d \right) \right] \\ &\quad + \frac{1}{2}d^2\widehat{V}(0) + \delta\lambda^{\min} \\ &\geq \inf_{(\gamma,\alpha)\in\mathcal{D}'} \left[ \mathcal{F}^{\text{aux}}(\gamma, \alpha, \rho_0^{\min} + d) - \delta \int \gamma \right] + \delta(\lambda^{\min} - d) \\ &\quad + \frac{1}{2}d^2\widehat{V}(0), \end{aligned}$$

where we have also used that $(\tilde{\gamma}_\varepsilon, \tilde{\alpha}_\varepsilon) \in \mathcal{D}'$ for all $\varepsilon$. By taking a supremum over $\delta$ on both sides and using (4.32), we obtain

$$F^{\text{aux}}(\lambda^{\min}, \rho_0^{\min}) \geq F^{\text{aux}}(\lambda^{\min} - d, \rho_0^{\min} + d) + \frac{1}{2}d^2\widehat{V}(0).$$

Thus, if $d > 0$ we arrive at a contradiction with the fact that $(\lambda^{\min}, \rho_0^{\min})$ is the minimum of $F^{\text{aux}}(\lambda, \rho_0)$ as $\widehat{V}(0) \geq 0$ . This means the case $\int \gamma < \lambda^{\min}$ cannot occur. Since we had already proved the claims for the other case, this concludes the proof of the proposition. □

We need a final lemma to show the existence of a minimizer for the dual auxiliary problem.

**Lemma 33.** *Let $(\gamma_\kappa, \alpha_\kappa)$ and $(\tilde{\gamma}, \tilde{\alpha})$ be as above. In particular, we have $\gamma_\kappa \to \tilde{\gamma}$ pointwise and in $L^1$, and $\alpha_\kappa \to \tilde{\alpha}$ pointwise. We then have*

$$\liminf_{\kappa\to\infty} \mathcal{F}^{\text{aux}}_{\delta^{\min}}(\gamma_\kappa, \alpha_\kappa, \rho_0^{\min}) \geq \mathcal{F}^{\text{aux}}_{\delta^{\min}}(\tilde{\gamma}, \tilde{\alpha}, \rho_0^{\min}).$$

*Proof.* We recall that

$$\begin{aligned}\mathcal{F}^{\text{aux}}_{\delta^{\min}}(\gamma,\alpha,\rho_0^{\min}) = &\int p^2\gamma(p)dp - T\int s(\gamma(p),\alpha(p))dp - \delta^{\min}\int \gamma(p)dp \\ &+\rho_0^{\min}\int \widehat{V}(p)(\gamma(p)+\alpha(p))dp \\ &+\frac{1}{2}\int\int \widehat{V}(p-q)(\gamma(p)\gamma(q)+\alpha(p)\alpha(q))dpdq.\end{aligned} \tag{4.33}$$

The third term on the right-hand side simply converges because of the $L^1$-convergence of the $\gamma_\kappa$. The combination of the first two terms is bounded below by an integrable function (as in (3.8)) and thus we can use pointwise convergence in combination with Fatou's lemma to conclude

$$\int p^2\tilde{\gamma} - T\int s(\tilde{\gamma},\tilde{\alpha}) \le \liminf_{\kappa\to\infty}\left(\int p^2\gamma_\kappa - T\int s(\gamma_\kappa,\alpha_\kappa)\right).$$

To show that the fourth term in (4.33) also converges, we use two estimates. The easier one is

$$\left|\rho_0^{\min}\int \widehat{V}\,(\gamma_\kappa-\tilde{\gamma})\right| \le \rho_0^{\min}\|\widehat{V}\|_\infty\int|\gamma_\kappa-\tilde{\gamma}|, \tag{4.34}$$

which goes to zero by the $L^1$-convergence of the $\gamma_\kappa$. For the term involving $\tilde{\alpha}$, we write for $\varepsilon>0$

$$\int_{|p|\le\varepsilon}|\alpha_\kappa| = \int_{|p|\le\varepsilon,|\gamma_\kappa|\le1}|\alpha_\kappa| + \int_{|p|\le\varepsilon,|\gamma_\kappa|>1}|\alpha_\kappa| \quad \le C\varepsilon^3+\sqrt{2}\int_{|p|\le\varepsilon}\gamma_\kappa,$$

where we have used the usual estimate on $\alpha_\kappa$ in terms of $\gamma_\kappa$. Note that this also holds for $\tilde{\alpha}$ (in terms of $\tilde{\gamma}$). For $|p|>\varepsilon$ and $\kappa$ large enough we see from $|\alpha_\kappa|^2\le\gamma_\kappa(\gamma_\kappa+1)$ and Lemmas 24 and 27 that the Dominated Convergence Theorem gives

$$\lim_{\kappa\to\infty}\int_{|p|>\varepsilon}|\tilde{\alpha}-\alpha_\kappa|^2=0.$$

Hence

$$\begin{aligned}\int|\widehat{V}||\tilde{\alpha}-\alpha_\kappa| &\le \|\widehat{V}\|_\infty\int_{|p|\le\varepsilon}|\tilde{\alpha}-\alpha_\kappa| + \int_{|p|>\varepsilon}|\widehat{V}||\tilde{\alpha}-\alpha_\kappa| \\ &\le \|\widehat{V}\|_\infty\int_{|p|\le\varepsilon}(|\tilde{\alpha}|+|\alpha_\kappa|) + \left(\int_{|p|>\varepsilon}|\widehat{V}|^2\right)^{\frac12}\left(\int_{|p|>\varepsilon}|\tilde{\alpha}-\alpha_\kappa|^2\right)^{\frac12} \\ &\le C\|\widehat{V}\|_\infty\varepsilon^3+\sqrt{2}\|\widehat{V}\|_\infty\int_{|p|\le\varepsilon}(\gamma_\kappa+\tilde{\gamma}) + C\left(\int_{|p|>\varepsilon}|\tilde{\alpha}-\alpha_\kappa|^2\right)^{\frac12} \\ &\xrightarrow{\kappa\to\infty}\quad C\|\widehat{V}\|_\infty\varepsilon^3+2\sqrt{2}\|\widehat{V}\|_\infty\int_{|p|\le\varepsilon}\tilde{\gamma}.\end{aligned} \tag{4.35}$$

Since this holds for any $\varepsilon>0$ and tends to 0 as $\varepsilon\to0$, we combine our conclusion with the first estimate to see that the entire third term converges, i.e.

$$\rho_0^{\min}\int\widehat{V}(p)\left(\gamma_\kappa(p)+\alpha_\kappa(p)\right)dp \to \rho_0^{\min}\int\widehat{V}(p)\left(\tilde{\gamma}(p)+\tilde{\alpha}(p)\right)dp.$$

Finally, we need to take care of the fifth term in (4.33). It is enough to bound

$$\left|\sqrt{\iint \tilde{\gamma}(p)\widehat{V}(p-q)\tilde{\gamma}(q)dpdq}-\sqrt{\iint \gamma_\kappa(p)\widehat{V}(p-q)\gamma_\kappa(q)dpdq}\right| \tag{4.36}$$
$$\leq \sqrt{\iint (\gamma_\kappa(p)-\tilde{\gamma}(p))\widehat{V}(p-q)(\gamma_\kappa(q)-\tilde{\gamma}(q))dpdq} \leq \|\hat{V}\|_\infty^{1/2}\|\gamma_\kappa-\tilde{\gamma}\|_1,$$

where we have used that $V \geq 0$. This implies convergence of the $\gamma$-part of the fifth term. Since we do not have $L^1$-convergence for $\alpha_\kappa$, we need to use a different method. We again need to control

$$\begin{aligned}&\iint (\alpha_\kappa-\tilde{\alpha})(p)\widehat{V}(p-q)(\alpha_\kappa-\tilde{\alpha})(q)dpdq\\ &\leq 2\iint_{|p|,|q|>\varepsilon}(\alpha_\kappa-\tilde{\alpha})(p)\widehat{V}(p-q)(\alpha_\kappa-\tilde{\alpha})(q)dpdq\\ &\quad +2\iint_{|p|,|q|<\varepsilon}(\alpha_\kappa-\tilde{\alpha})(p)\widehat{V}(p-q)(\alpha_\kappa-\tilde{\alpha})(q)dpdq.\end{aligned}$$

For the first integral we use

$$\begin{aligned}&\int_{|p|,|q|>\varepsilon}(\alpha_\kappa-\tilde{\alpha})(p)\widehat{V}(p-q)(\alpha_\kappa-\tilde{\alpha})(q)dpdq =\\ &\quad = \int V(x)|\mathcal{F}^{-1}\left((\alpha_\kappa-\tilde{\alpha})\mathbb{1}(|p|>\varepsilon)\right)|^2dx \qquad (4.37)\\ &\quad \leq \|V\|_\infty\|\mathcal{F}^{-1}\left((\alpha_\kappa-\tilde{\alpha})\,\mathbb{1}(|p|>\varepsilon)\right)\|_2^2 = \|V\|_\infty\int_{|p|>\varepsilon}|\alpha_\kappa-\tilde{\alpha}|^2,\end{aligned}$$

where $\mathcal{F}^{-1}$ denotes the inverse Fourier transform. The second integral is bounded by

$$\begin{aligned}\int\limits_{|p|,|q|\leq\varepsilon}(\alpha_\kappa-\tilde{\alpha})(p)\widehat{V}(p-q)(\alpha_\kappa-\tilde{\alpha})(q)dpdq &\leq \|V\|_1\left(\int\limits_{|p|\leq\varepsilon}|\alpha_\kappa-\tilde{\alpha}|dp\right)^2 \qquad (4.38)\\ &\leq \|V\|_1\left(C\varepsilon^3+C\int_{|p|\leq\varepsilon}(\gamma_\kappa+\tilde{\gamma})\right)^2,\end{aligned}$$

where we used the same bound as in the first term of (4.35). Taking the limit $\kappa\to\infty$ followed by $\varepsilon\to 0$ in (4.37), (4.38) and the bound above, we see that we have convergence of the $\alpha$-part of the fifth term. This concludes the proof of the lemma. □

We are ready to prove the main statement of this subsection.

*Proof of Theorem 29.* We combine the previous two lemmas to obtain

$$\begin{aligned}\inf_{(\gamma,\alpha)\in\mathcal{D}'}\mathcal{F}^{\text{aux}}_{\delta^{\min}}(\gamma,\alpha,\rho_0^{\min}) &= \liminf_{\kappa\to\infty}\mathcal{F}^{\text{aux}}_{\delta^{\min}}(\gamma_\kappa,\alpha_\kappa,\rho_0^{\min}) \geq \mathcal{F}^{\text{aux}}_{\delta^{\min}}(\tilde{\gamma},\tilde{\alpha},\rho_0^{\min})\\ &\geq \inf_{(\gamma,\alpha)\in\mathcal{D}'}\mathcal{F}^{\text{aux}}_{\delta^{\min}}(\gamma,\alpha,\rho_0^{\min}),\end{aligned}$$

where the first equality holds by Lemma 31 and the first inequality holds by Lemma 33. We conclude that the $(\tilde{\gamma}, \tilde{\alpha})$ constructed in Proposition 32 has to be a minimizer. Indeed,

$$\mathcal{F}^{\text{aux}}_{\delta^{\min}}(\tilde{\gamma}, \tilde{\alpha}, \rho_0^{\min}) = \inf_{(\gamma,\alpha)\in\mathcal{D}'} \mathcal{F}^{\text{aux}}_{\delta^{\min}}(\gamma, \alpha, \rho_0^{\min}) = \hat{F}^{\text{aux}}\left(\delta^{\min}, \rho_0^{\min}\right)$$

which concludes the proof. □

*Remark* 34. The statement remains true in one and two dimensions.

## 5. Existence of minimizers for $T = 0$

In this section, we prove Theorems 2 and 5. The proof of the existence of minimizers for $T > 0$ relied upon the bounds derived in Section 4.4. These showed that the minimizers of the restricted problem are uniformly bounded for fixed $T$, which allowed us to extract a limit. However, the bound deteriorates as $T \to 0$ and hence the proof cannot be used for $T = 0$. In this section we prove the existence of a minimizer for $T = 0$ in a different way.

5.1. **The grand canonical case.** We first consider the grand canonical functional. Note that the statement is trivial for $T = 0$ and $\mu \leq 0$, since in this case the functional is obtained by taking expectation values of a positive operator. The minimizer is given by the vacuum, i.e. $(\gamma, \alpha, \rho_0) = (0, 0, 0)$.

The rest of this subsection is dedicated to proving the theorem for $\mu > 0$. By the main result of the previous section, we know that for any $\mu$ and $T > 0$ there exists a minimizer of the grand canonical functional (1.1). In this section, we will denote this functional as $\mathcal{F}^T$ to make the $T$-dependence explicit. As the proposition below shows, its minimizers at temperature $T$ actually form a minimizing sequence as $T \to 0$ for the $T = 0$ case.

**Proposition 35** ($T = 0$ minimizing sequence)**.** *Let $(\gamma^T, \alpha^T, \rho_0^T)$ be a minimizer for $F(T, \mu)$ with $\mu, T > 0$. Then*

$$TS(\gamma^T, \alpha^T) \xrightarrow{T\to 0} 0 \quad \textit{and} \quad \mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T) \xrightarrow{T\to 0} F(0, \mu).$$

*Proof.* Let $T_1 < T_2$. Making use of the minimizers at these temperatures, we obtain

$$\begin{aligned}
\mathcal{F}^{T_1}(\gamma^{T_1}, \alpha^{T_1}, \rho_0^{T_1}) &= \mathcal{F}^0(\gamma^{T_1}, \alpha^{T_1}, \rho_0^{T_1}) - T_1 S(\gamma^{T_1}, \alpha^{T_1}) \\
&\leq \mathcal{F}^0(\gamma^{T_2}, \alpha^{T_2}, \rho_0^{T_2}) - T_1 S(\gamma^{T_2}, \alpha^{T_2}) \\
&= \mathcal{F}^0(\gamma^{T_2}, \alpha^{T_2}, \rho_0^{T_2}) - T_2 S(\gamma^{T_2}, \alpha^{T_2}) + (T_2 - T_1) S(\gamma^{T_2}, \alpha^{T_2}) \\
&\leq \mathcal{F}^0(\gamma^{T_1}, \alpha^{T_1}, \rho_0^{T_1}) - T_2 S(\gamma^{T_1}, \alpha^{T_1}) + (T_2 - T_1) S(\gamma^{T_2}, \alpha^{T_2}).
\end{aligned}$$

Comparing the first and last line we see that $S(\gamma^{T_1}, \alpha^{T_1}) \leq S(\gamma^{T_2}, \alpha^{T_2})$, and thus the entropy of the minimizers decreases when $T$ does. Since it has to be non-negative, this implies that $TS(\gamma^T, \alpha^T) \to 0$ as $T \to 0$.

Now, note that for all $(\gamma, \alpha, \rho_0) \in \mathcal{D}$ one has

$$\mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T) - TS(\gamma^T, \alpha^T) \leq \mathcal{F}^0(\gamma, \alpha, \rho_0) - TS(\gamma, \alpha).$$

Taking a $\limsup_{T\to 0}$ followed by an infimum over $(\gamma, \alpha, \rho_0)$ and combining this with

$$\liminf_{T\to 0} \mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T) \geq F(0, \mu),$$

proves the second claim. $\square$

Now that we know that $\{(\gamma^T, \alpha^T, \rho_0^T)\}_{\{T>0\}}$ is a minimizing sequence, we would like to extract a limit out of it. This can in fact be done.

**Proposition 36.** *There exists a subsequence of* $\{(\gamma^T, \alpha^T, \rho_0^T)\}_{\{T>0\}}$ *such that* $\gamma^T \to \tilde{\gamma}$ *pointwise and in* $L^1$*,* $\alpha^T \to \tilde{\alpha}$ *pointwise and in* $L^2$*, and* $\rho_0^T \to \tilde{\rho}_0$*. Moreover, the limit is an admissible state, i.e.* $(\tilde{\gamma}, \tilde{\alpha}, \tilde{\rho}_0) \in \mathcal{D}$*.*

We will first state the proof of Theorem 2. The rest of this section will then be dedicated to proving Proposition 36.

*Proof of Theorem 2.* As mentioned at the beginning of this section, the functional with $\mu \leq 0$ has a minimizer $\gamma = \alpha = \rho_0 = 0$, so there is nothing left to prove. We consider the case $\mu > 0$. By Proposition 36, we can assume that a suitable subsequence of $(\gamma^T, \alpha^T, \rho_0^T)$ has the convergence properties stated. Let us recall what the relevant functional looks like:

$$\begin{aligned}\mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T) = &\int p^2\gamma^T(p)dp - \mu\rho^T + \frac{1}{2}\widehat{V}(0)\left(\rho^T\right)^2\\ &+ \rho_0^T \int \widehat{V}(p)(\gamma^T(p) + \alpha^T(p))dp\\ &+ \frac{1}{2}\int \widehat{V}(p-q)\left[\alpha^T(p)\alpha^T(q) + \gamma^T(p)\gamma^T(q)\right] dpdq.\end{aligned}$$

We will show that this converges to something that is bigger than or equal to $\mathcal{F}^0(\tilde{\gamma}, \tilde{\alpha}, \tilde{\rho}_0)$, much like in Lemma 33. The first term can be treated by Fatou's lemma and pointwise convergence (see (4.24) for a similar application). The second and third terms simply converge since $\rho_0^T \to \tilde{\rho}_0$ and $\rho_\gamma^T \to \rho_{\tilde{\gamma}}$ by $L^1$-convergence. The remaining terms involving $\gamma^T$ converge because of $L^1$-convergence (see estimates (4.34) and (4.36)). The quadratic $\alpha^T$-term is taken care of using $L^2$-convergence and the estimate (4.37), where now the integrals are over all $p$ and $q$. $L^2$-convergence also suffices to show convergence of the term linear in $\alpha^T$:

$$\left|\int \widehat{V}\tilde{\alpha} - \int \widehat{V}\alpha^T\right| \leq \int \widehat{V}|\tilde{\alpha} - \alpha^T| \leq \left(\int |\widehat{V}|^2\right)^{1/2} \left(\int |\tilde{\alpha} - \alpha^T|^2\right)^{1/2}.$$

We have thus shown that

$$\liminf_{T\to 0} \mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T) \geq \mathcal{F}^0(\tilde{\gamma}, \tilde{\alpha}, \tilde{\rho}_0).$$

Together with Proposition 35, this leads to

$$F(0,\mu) = \liminf_{T\to 0} \mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T) \geq \mathcal{F}^0(\tilde{\gamma}, \tilde{\alpha}, \tilde{\rho}_0) \geq F(0, \mu),$$

which proves that $(\tilde{\gamma}, \tilde{\alpha}, \tilde{\rho}_0)$ is indeed a minimizer. $\square$

It remains to prove Proposition 36. As mentioned before, some bounds in Section 4.4 cannot be obtained uniformly in $T$, so they are useless for this case. However, the equivalent of Lemma 24 (with $\mu$ rather than $\delta$) does hold uniformly.

**Lemma 37.** *Let $\mu \in \mathbb{R}$. There exist $C, P_0, T_0 > 0$ such that for all $|p| > P_0$ and $0 < T \leq T_0$, we have*

$$\gamma^T(p) \leq C|p|^{-4}.$$

We also need the following lemma.

**Lemma 38.** *For every $\mu > 0$, there exists a temperature $T_1 > 0$, such that any minimizer of the grand canonical functional* (1.1) *at temperatures $0 \leq T \leq T_1$ and chemical potential $\mu$ has $\rho_0 > 0$.*

*Proof.* Assume that a minimizer has $\rho_0 = 0$. This implies that its $\gamma$ satisfies

$$\mathcal{F}^T(\gamma, 0, 0) \leq \inf_{\rho_0} \mathcal{F}^T(0, 0, \rho_0) = \frac{-\mu^2}{2\widehat{V}(0)}, \tag{5.1}$$

since adding an $\alpha$ could only raise the energy (due to the monotonicity of the entropy (3.1)). We have

$$\mathcal{F}^T(\gamma, 0, 0) = \frac{1}{2}\int p^2\gamma(p)dp + \frac{1}{2}\int \widehat{V}(p-q)\gamma(p)\gamma(q)dpdq \tag{5.2}$$

$$+ \frac{1}{2}\widehat{V}(0)\rho_\gamma^2 - \mu\rho_\gamma \tag{5.3}$$

$$+ \frac{1}{2}\int p^2\gamma(p)dp - TS(\gamma, 0). \tag{5.4}$$

Clearly,

$$(5.3) \geq \frac{-\mu^2}{2\widehat{V}(0)}, \tag{5.5}$$

and (5.4) can be bounded as in (3.8), i.e.

$$(5.4) \geq -CT^{5/2}, \tag{5.6}$$

where $C$ is a positive constant. Since $\widehat{V}(0) > 0$ and $\widehat{V} \in C^1$, we can pick $p_0 > 0$ small enough such that $\min_{|p|\leq 2p_0} \widehat{V}(p) > 0$, and

$$(5.2) \geq \frac{1}{2}p_0^2 \int_{|p|>p_0} \gamma(p)dp + \frac{1}{2}\left(\min_{|p|\leq 2p_0} \widehat{V}(p)\right)\left(\int_{|p|\leq p_0} \gamma(p)dp\right)^2.$$

The last expression can be minimized in $\int_{|p|\leq p_0}\gamma$, where we also take into account that it is less than $\rho_\gamma$. The lower bounds we deduce are

$$\begin{array}{lll} \frac{1}{2}\min_{|p|\leq 2p_0}\widehat{V}(p)\rho_\gamma^2 & \text{if} & \rho_\gamma \leq \dfrac{p_0^2}{2\min_{|p|\leq 2p_0}\widehat{V}(p)} \\ \frac{1}{4}p_0^2\rho_\gamma & \text{if} & \rho_\gamma > \dfrac{p_0^2}{2\min_{|p|\leq 2p_0}\widehat{V}(p)}. \end{array}$$

It follows that there exist $c_1, c_2 > 0$ depending only on $V$ such that

$$(5.2) \geq \min\{c_1\rho_\gamma, c_2\rho_\gamma^2\}. \tag{5.7}$$

Putting together (5.1), (5.5), (5.6) and (5.7), we see that any minimizer with $\rho_0 = 0$ has to satisfy

$$\min\{c_1\rho_\gamma, c_2\rho_\gamma^2\} \leq CT^{5/2}.$$

However, this means that there exist $c_3, c_4 > 0$ depending only on $V$ such that

$$\begin{aligned}\frac{\partial\mathcal{E}(\gamma,0,\rho_0)}{\partial\rho_0}\Big|_{\rho_0=0} &= -\mu + \widehat{V}(0)\int\gamma + \int\widehat{V}\gamma \leq -\mu + 2\widehat{V}(0)\int\gamma \\ &\leq -\mu + \max\{c_3T^{5/2}, c_4T^{5/4}\}.\end{aligned} \tag{5.8}$$

This implies the existence of a temperature $T_1$ depending on $\mu$ and $V$ such that this derivative is negative for all $0 \leq T \leq T_1$, which means that there cannot be minimizers with $\rho_0 = 0$. □

*Proof of Proposition 36.* We split the proof into several steps in which we obtain the different limits. For simplicity we use the notation $\int\gamma^T =: \rho_\gamma^T$ and $\rho^T := \rho_\gamma^T + \rho_0^T$.

*Step 1: Limit for $\rho_0^T$ and $\rho_\gamma^T$.* We will show that both these sequences are uniformly bounded. Since we are dealing with minimizers, we have

$$\frac{-\mu^2}{2\widehat{V}(0)} = \mathcal{F}^T\left(0,0,\frac{\mu}{\widehat{V}(0)}\right) \geq \mathcal{F}^0\left(\gamma^T,\alpha^T,\rho_0^T\right) - TS(\gamma^T,\alpha^T).$$

Since by Proposition 35 the entropy term converges to 0 as $T \to 0$, for $T$ small enough we have

$$\begin{aligned}\frac{-\mu^2}{4\widehat{V}(0)} &\geq -\mu\rho^T + \frac{1}{2}\widehat{V}(0)\left(\rho^T\right)^2 + \rho_0^T\int\widehat{V}(\gamma^T+\alpha^T) \\ &\geq \rho_0^T(-\mu - \frac{1}{2}\int\widehat{V}) + \frac{1}{2}\widehat{V}(0)\left(\rho_0^T\right)^2 - \mu\rho_\gamma^T + \frac{1}{2}\widehat{V}(0)\left(\rho_\gamma^T\right)^2,\end{aligned}$$

where we have thrown out some positive terms and used the fact that $\gamma + \alpha \geq -\frac{1}{2}$. This estimate implies that $\rho_0^T$ and $\rho_\gamma^T$ are uniformly bounded. We can extract a limit by taking subsequences, so that from now on we have $\rho_0^T \to \tilde{\rho}_0$ and $\rho_\gamma^T \to \tilde{\rho}_\gamma$.

*Step 2: Limit for $\int\widehat{V}(\gamma^T+\alpha^T)$ and $\tilde{\rho}_0 > 0$.* It follows from Lemma 38 that $\rho_0^T > 0$ for $T$ small enough. This implies that the Euler–Lagrange equation in $\rho_0$ has to hold with equality for $T$ small enough:

$$-\mu + \int\widehat{V}(\gamma^T+\alpha^T) + \widehat{V}(0)\rho^T = 0. \tag{5.9}$$

Since we know that $\rho^T$ has a limit as $T \to 0$, the integral in the equation above will also have a limit.

We now consider the following trial state:

$$\gamma = \gamma_0 \mathbb{1}_{B_\varepsilon}$$
$$\alpha = -\sqrt{(\gamma_0(\gamma_0+1)} \mathbb{1}_{B_\varepsilon},$$

where $B_\varepsilon$ denotes the ball with radius $\varepsilon$ (which will be fixed later) centred at the origin. We have

$$\mathcal{F}^0\left(\gamma, \alpha, \mu(\widehat{V}(0))^{-1} - \gamma_0|B_\varepsilon|\right) - \mathcal{F}^0\left(0,0,\mu(\widehat{V}(0))^{-1}\right) =$$

$$= \gamma_0 \int_{B_\varepsilon} p^2 dp + \left(\frac{\mu}{\widehat{V}(0)} - |B_\varepsilon|\gamma_0\right)(\gamma_0 - \sqrt{(\gamma_0(\gamma_0+1))}) \int_{B_\varepsilon} \widehat{V}(p)dp \tag{5.10}$$
$$+ \frac{2\gamma_0^2+\gamma_0}{2} \iint_{B_\varepsilon \times B_\varepsilon} \widehat{V}(p-q)dpdq.$$

Assume that $\gamma_0$ is large enough, in particular $\gamma_0 > 1$. Then

$$\gamma_0 - \sqrt{(\gamma_0(\gamma_0+1)} = -\frac{1}{2} + O(\gamma_0^{-1}).$$

We also choose the radius $\varepsilon$ in such a way that

$$|B_\varepsilon| = \frac{\nu}{\gamma_0^2}$$

for a positive constant $\nu$. The fact that $\widehat{V} \in C^1$ and $\widehat{V}(0) > 0$ imply that $\widehat{V}(p) \geq \frac{1}{2}\widehat{V}(0)$ on $B_\varepsilon$ for $\gamma_0$ large enough. It follows that

$$(5.10) \leq C\gamma_0|B_\varepsilon|^{5/3} - (\frac{1}{2} - O(\gamma_0^{-1}))\left(\frac{\mu}{\widehat{V}(0)} - |B_\varepsilon|\gamma_0\right)|B_\varepsilon|\frac{\widehat{V}(0)}{2}$$
$$+ \widehat{V}(0)|B_\varepsilon|^2\frac{2\gamma_0^2+\gamma_0}{2},$$

where $C$ is a positive constant. Hence, for $\nu < \frac{\mu}{4\widehat{V}(0)}$ and $\gamma_0$ sufficiently large

$$(5.10) \leq C\gamma_0^{-7/3} - \frac{1}{2}\left(\frac{\widehat{V}(0)}{2} - O(\gamma_0^{-1})\right)\left(\frac{\mu}{\widehat{V}(0)} - \frac{\nu}{\gamma_0}\right)\frac{\nu}{\gamma_0^2} + \widehat{V}(0)\nu^2\frac{2\gamma_0^2+\gamma_0}{2\gamma_0^4}$$
$$= \left(\nu\widehat{V}(0) - \frac{\mu}{4}\right)\frac{\nu}{\gamma_0^2} + o(\gamma_0^{-2}) < 0.$$

Also note that $\gamma_0 > 1$ implies $\mu(\widehat{V}(0))^{-1} - \gamma_0|B_\varepsilon| \geq 0$, which means that our choice of $\rho_0$ in (5.10) was allowed.

Together with Proposition 35, this calculation implies that

$$\frac{-\mu^2}{2\widehat{V}(0)} > F(0,\mu) = \lim_{T\to 0} \mathcal{F}^0(\gamma^T, \alpha^T, \rho_0^T)$$
$$= \lim_{T\to 0}\left[\int p^2\gamma^T + \frac{1}{2}\int \widehat{V}(p-q)\left[\alpha^T(p)\alpha^T(q) + \gamma^T(p)\gamma^T(q)\right]dpdq\right]$$
$$+ \left[-\mu\tilde{\rho} + \frac{1}{2}\widehat{V}(0)\tilde{\rho}^2\right] + \tilde{\rho}_0 \lim_{T\to 0}\int \widehat{V}(\gamma^T + \alpha^T). \tag{5.11}$$

The first limit has to be non-negative and the term involving $\tilde{\rho}$ has to be bigger than or equal to $-\mu^2/2\widehat{V}(0)$. We therefore conclude that

$$\begin{aligned} \tilde{\rho}_0 &> 0, \\ \lim_{T\to 0}\int \widehat{V}(\gamma^T+\alpha^T) &= -C < 0. \end{aligned} \tag{5.12}$$

*Step 3: Limits for $TA^T$ and $TB^T$.* Recall from Section 4.4 that the Euler–Lagrange equations of the functional lead to an expression for $\gamma^T$ in terms of the functions

$$\begin{aligned} TA^T(p) &= p^2-\mu+\widehat{V}(0)\rho^T+\rho_0^T\widehat{V}(p)+\widehat{V}*\gamma^T(p), \\ TB^T(p) &= \rho_0^T\widehat{V}(p)+\widehat{V}*\alpha^T(p), \\ TG^T(p) &= \sqrt{(TA^T(p))^2-(TB^T(p))^2}. \end{aligned} \tag{5.13}$$

We will establish a limit for these functions, and then prove that it leads to a limit for $\gamma^T$. Note that we only need to deal with the convolution terms since all other terms already have a limit or are constant in $T$.

Our goal is a pointwise limit on the whole space, and a $C^2$-limit on the compact $\{|p|\leq P_0\}$, where $P_0$ is given by Lemma 37. Recall our assumption that $\widehat{V}$ is in $C^3(\mathbb{R}^3)$ and that all its derivatives up to third order are bounded. This implies that $\widehat{V}*\gamma^T$ and $\widehat{V}*\alpha^T$ are also in $C^3(\mathbb{R}^3)$ and, using the bounds (3.7) on these quantities and the uniform bound on $\rho_\gamma^T$, that all derivatives up to third order are uniformly bounded in $T$. In particular, $\widehat{V}*\gamma^T$ and $\widehat{V}*\alpha^T$ are uniformly bounded with uniformly bounded derivatives, and the latter implies uniform equicontinuity. All this means that by a diagonal argument one can construct a pointwise limit on $\mathbb{R}^3$ (that is continuous) by selecting subsequences that converge on the rationals (see, e.g. Theorem I.26 in [25]). By the Arzelà–Ascoli theorem, this implies that taking further subsequences leads to a uniform limit on the compact $\{|p|\leq P_0\}$. We now repeat this last argument for the derivatives and second-order derivatives on $\{|p|\leq P_0\}$. We obtain uniform (continuous) limits for all derivatives up to second order. By uniform convergence these are indeed derivatives of the limit functions.

Summarizing, we have obtained limits $a$ and $b$ that are bounded and in $C^2(|p|\leq P_0)$ such that $TA^T\to a$ and $TB^T\to b$ pointwise and also uniformly on $\{|p|\leq P_0\}$. We also note that by (5.9), (5.12) and (5.13): $a\geq C>0$. By the Euler–Lagrange equations for $T>0$ we have $|TB^T|\leq TA^T$, so the limits also satisfy $|b|\leq a$. Hence $TG^T$ also has a pointwise limit $g=\sqrt{a^2-b^2}$ that is a bounded function.

*Step 4: Limit for $\gamma^T$.* As in Section 4.4 we derive an expression for $\gamma^T$ in terms of $A^T$ and $G^T$ given by (5.13). To make use of the limits we have obtained, we write it as follows:

$$\gamma^T=\frac{TA^T-TG^T+e^{-\frac{1}{T}(TG^T)}\left(TA^T+TG^T\right)}{2TG^T\left(1-e^{-\frac{1}{T}(TG^T)}\right)}. \tag{5.14}$$

We conclude that pointwise

$$\gamma^T \xrightarrow{T\to 0} \frac{a-g}{2g} =: \tilde{\gamma}, \tag{5.15}$$

which is easy to see when $g > 0$, but since $a > 0$ it is also true for $g = 0$ (with the understanding that $\gamma^T = +\infty$ at such points). We would nonetheless like to prove that $g = 0$ actually cannot happen.

First note that $g(p)$ is bounded away from 0 for $|p| \geq P_0$ by the bound in Lemma 37 and the fact that $a \geq C > 0$. Now suppose that $g^2(p_0) = (a^2 - b^2)(p_0) = 0$ for some $|p_0| < P_0$. We know that $a^2$ and $b^2$ are $C^2$ around $p_0$ and that $b^2 \leq a^2$. Therefore, $a^2 - b^2$ has to behave like $(p-p_0)^2 + o(p-p_0)^2$ around $p_0$. Since $a \geq C > 0$, we see that $\tilde{\gamma}$ has to go to infinity like $|p-p_0|^{-1}$ or faster. If we assume that $p_0 \neq 0$, this implies that $\tilde{\gamma}$ is non-integrable, which, by Fatou's lemma, contradicts the pointwise convergence:

$$\int \tilde{\gamma} \leq \liminf_{T\to 0} \int \gamma^T = \tilde{\rho}_\gamma < \infty.$$

We therefore conclude that $g(p)$ cannot be zero for $p \neq 0$. However, using (5.9) and (5.13) we can calculate that

$$g(0) = \sqrt{(a(0)-b(0))(a(0)+b(0))} = \sqrt{-4\tilde{\rho}_0 \widehat{V}(0)\left[\lim_{T\to 0}\int \widehat{V}\alpha^T\right]} > 0,$$

where the inequality holds by (5.12). We can now conclude that $g \neq 0$. Since it is continuous, it has to be bounded away from zero on the compact $|p| \leq P_0$, and combined with our previous observation, everywhere.

We now analyse the expression (5.14) and conclude that the convergence (5.15) is actually uniform on $\{|p| \leq P_0\}$. For this we use the following facts: a sum preserves uniform convergence; a product preserves uniform convergence given that the limit functions are bounded; a composition $g \circ f_n$ preserves uniform convergence (of the $f_n$) if $g$ is uniformly continuous in the region where $f_n$ takes values. Since it is necessary to apply this last fact to the function $x \mapsto 1/x$, it is crucial that $g$ is bounded away from 0.

We can finally prove that $\gamma^T \to \tilde{\gamma}$ in $L^1$. The uniform convergence implies $L^1$-convergence on $\{|p| \leq P_0\}$. By Lemma 37, we have also uniform boundedness by an $L^1$-function on $\{|p| > P_0\}$. Applying the Dominated Convergence Theorem to that region, we conclude that $\gamma^T \to \tilde{\gamma}$ in $L^1$. The pointwise convergence obtained before also implies $\tilde{\gamma} \geq 0$, and by Fatou's lemma, $\int p^2 \tilde{\gamma} dp < \infty$.

*Step 5: Limit for $\alpha^T$.* As before, we use relations that are known to hold for $T > 0$ to conclude convergence:

$$\beta^T = \sqrt{\left(\gamma^T + \frac{1}{2}\right)^2 - (\alpha^T)^2} = \frac{1 + e^{-\frac{1}{T}(TG^T)}}{2(1 - e^{-\frac{1}{T}(TG^T)})} \xrightarrow{T\to 0} \frac{1}{2}$$

$$\alpha^T = -\beta^T \frac{TB^T}{TG^T} \xrightarrow{T\to 0} -\frac{b}{2g} =: \tilde{\alpha}.$$

Again, the convergence holds pointwise everywhere and uniformly on $\{|p| \leq P_0\}$. The uniform convergence implies $L^2$-convergence on $\{|p| \leq P_0\}$. Since

$\left(\alpha^T\right)^2 \leq \gamma^T(\gamma^T+1)$, Lemma 37 leads to an uniform $L^2$-bound on the $\alpha^T$ for $\{|p| \geq P_0\}$. Hence, $L^2$-convergence also holds in this region by the Dominated Convergence Theorem. Also note that $\beta^T \to 1/2$ implies that $\tilde{\alpha}^2 = \tilde{\gamma}(\tilde{\gamma}+1)$. We have now proved all the claims in the proposition. □

It remains to prove Corollary 6.

*Proof Corollary 6 for the grand canonical functional.* Our goal will be to show that any minimizer at $T=0$ has to satisfy $\alpha^2 = \gamma(\gamma+1)$ using elements from the proof above. The corollary then follows from Theorem 10.4 in [30], which states that the 1-pdm $\Gamma$ corresponds to pure quasi-free states if and only if

$$\Gamma \mathcal{S} \Gamma = -\Gamma$$

(cf. (A.3) and (A.2) for definitions). This is indeed satisfied if $\alpha^2 = \gamma(\gamma+1)$.

Note that $\mu \leq 0$ is easy, since the minimizer is $(\gamma, \alpha, \rho_0) = (0,0,0)$ as explained at the start of this section. For $\mu > 0$, we can consider (5.11) directly at $T=0$ (i.e. without the limits) to conclude that any minimizer has

$$\rho_0 > 0, \qquad \int \widehat{V}(\gamma+\alpha) < 0.$$

This implies that (5.9) holds, and so minimizers have

$$\frac{\partial \mathcal{F}}{\partial \gamma} = p^2 - \int \widehat{V}(\gamma+\alpha) + \rho_0 \widehat{V}(p) + \widehat{V} * \gamma(p) > 0,$$

which means that it is energetically favourable to lower $\gamma$ as much as possible. However, this can only be done up to the point where $\alpha^2 = \gamma(\gamma+1)$. □

5.2. **The canonical case.** We would now like to prove the existence of $T=0$ minimizers for the canonical problem. Recall that for fixed $\rho \geq 0$ and $T \geq 0$ the functional reads

$$\begin{aligned}\mathcal{F}^{\text{can}}(\gamma, \alpha, \rho-\rho_\gamma) = &\int p^2 \gamma(p) dp - TS(\gamma,\alpha) + \frac{1}{2}\widehat{V}(0)\rho^2 \\ &+ \left(\rho - \int \gamma\right) \int \widehat{V}(p)\left(\gamma(p)+\alpha(p)\right) dp \\ &+ \frac{1}{2} \iint \widehat{V}(p-q)\left(\alpha(p)\alpha(q) + \gamma(p)\gamma(q)\right) dp dq.\end{aligned}$$

*Proof of Theorem 5.* We follow the same strategy as in the grand canonical case. The same argument as in Proposition 35 implies that canonical, positive temperature minimizers at fixed $\rho$ form a minimizing sequence for the $T=0$ problem with that $\rho$.

We have

$$\begin{aligned}\frac{\partial \mathcal{F}^{\text{can}}}{\partial \gamma} &= p^2 + (\rho-\rho_\gamma)\widehat{V}(p) - \int \widehat{V}(\gamma+\alpha) + \widehat{V} * \gamma(p) - T\frac{\gamma+\frac{1}{2}}{\beta} \ln \frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}} \\ \frac{\partial \mathcal{F}^{\text{can}}}{\partial \alpha} &= (\rho-\rho_\gamma)\widehat{V}(p) + \widehat{V} * \alpha(p) + T\frac{\alpha}{\beta} \ln \frac{\beta+\frac{1}{2}}{\beta-\frac{1}{2}}.\end{aligned} \tag{5.16}$$

To see that these expressions are equal to zero for minimizers, we repeat the argument in Lemmas 22 and 23, but one extra ingredient is needed since

$\rho_\gamma \leq \rho$ provides an extra constraint compared to the grand canonical case. We therefore apply Theorem 9 (proved in the next section), which states that minimizers will have $\rho_0 > 0$ for sufficiently low temperatures. As a consequence, we arrive at the same bound as in Lemma 37.

We now repeat the proof of Proposition 36. Step 1 simplifies since $\rho_\gamma^T \leq \rho$ provides the required bound. For step 2, we first note that there is no equivalent to (5.9) in this case, but we can take a further subsequence to ensure that $\int \widehat{V}(\gamma^T + \alpha^T)$ has a limit. We then repeat the trial state argument (with $\mu/\widehat{V}(0)$ replaced with $\rho$), and it leads to the same conclusion as in the grand canonical case, that is

$$\tilde{\rho}_0 := \lim_{T\to 0}(\rho - \rho_\gamma^T) > 0,$$
$$\lim_{T\to 0}\int \widehat{V}(\gamma^T + \alpha^T) = -C < 0.$$

The canonical $TA^T$ reads

$$TA^T = p^2 + \rho_0^T \widehat{V}(p) - \int \widehat{V}(\gamma^T + \alpha^T) + \widehat{V} * \gamma^T(p),$$

which is really the same as (5.9) combined with (5.13). We then repeat the remaining steps in the proof of Proposition 36 to reach similar conclusions. To finish, we proceed as in the proof of Theorem 2. The conclusion of Corollary 6 for the canonical functional follows in an identical way. □

## 6. Phase transition and the grand canonical phase diagram

We start by proving Theorem 7, which states that there is only one kind of phase transition in the system. This holds for both the canonical and the grand canonical functional.

*Proof of Theorem 7. Step 1.* Let $T > 0$. Since

$$\int \widehat{V}(p-q)\alpha(p)\alpha(q)dpdq = \int V(x)|\check{\alpha}(x)|^2 dx \geq 0,$$

and $S(\gamma,\alpha) < S(\gamma,0)$ for $\alpha \not\equiv 0$, we directly see from the definition of the functionals (1.1) and (1.3) that $\rho_0 = 0$ implies $\alpha \equiv 0$.

Let $T > 0$. Recall from the proof of the existence of minimizers that the Euler–Lagrange equation for $\alpha$ is satisfied:

$$\int \widehat{V}(p-q)\alpha(q)dq + \rho_0\widehat{V}(p) + T\frac{\alpha(p)}{\beta(p)}\ln\frac{\beta(p)+\frac{1}{2}}{\beta(p)-\frac{1}{2}} = 0$$

for both functionals. Thus $\alpha \equiv 0$ implies $\rho_0 = 0$ as long as $\widehat{V}(p) > 0$ on some set of positive measure, which is the case since $\widehat{V}(0) > 0$ and $\widehat{V} \in C^1$.

*Step 2.* Let $T = 0$. For $\mu < 0$ (grand canonically) or $\rho = 0$ (canonically), we know that the minimizers have $\rho_0 = \alpha = 0$, so there is nothing to prove.

For $\mu > 0$ or $\rho > 0$, we know that $\rho_0 > 0$ by Theorems 8 and 9 respectively. Grand canonically, we have shown in Corollary 6 that $\alpha \not\equiv 0$, which followed from the trial state argument in step 2 of the proof of Proposition 36. As pointed out in the proof of Theorem 5, a similar argument can be done for the canonical case, and we again find $\alpha \not\equiv 0$. □

We now prove that there indeed exists a phase transition in the model.

*Proof of Theorem 8.* Note that the second part of the statement is proved in Lemma 38. It remains to show that there is no condensation for high temperatures.

The proof is based on two inequalities: an upper and a lower bound. The upper bound shows that for sufficiently large $T$ there exists a positive constant $C$ depending on $\mu$ and $V$ such that

$$\inf_{\gamma} \mathcal{F}(\gamma, 0, 0) \leq -CT^2 \ln T + O(T^2). \tag{6.1}$$

The lower bound shows that any minimizer $(\gamma, \alpha, \rho_0)$ with $\rho_0 > 0$ has to satisfy

$$\mathcal{F}(\gamma, \alpha, \rho_0) \geq -\tilde{C} T \ln T + O(T)$$

for sufficiently large $T$ and $\tilde{C}$ depending on $\mu$ and $V$. Hence, the minimizer has $\rho_0 = 0$ and $\alpha \equiv 0$ for $T$ large enough.

*Upper bound.* We start by proving (6.1). Note that

$$\mathcal{F}(\gamma, 0, 0) \leq \int (p^2 - \mu)\gamma(p) dp + \widehat{V}(0)\rho_\gamma^2 + T \int [\gamma(p) \ln \gamma(p) - (\gamma(p) + 1) \ln(\gamma(p) + 1)]\, dp.$$

To obtain an upper bound, we evaluate the right-hand side of the inequality above using the trial state

$$\gamma_\delta(p) = \left(e^{\frac{p^2+\delta}{T}} - 1\right)^{-1},$$

where $\delta$ is a positive constant, so that

$$\mathcal{F}(\gamma_\delta, 0, 0) \leq T \int \ln\left(1 - e^{\frac{-(p^2+\delta)}{T}}\right) dp - (\mu + \delta) \int \left(e^{\frac{p^2+\delta}{T}} - 1\right)^{-1} dp + \widehat{V}(0) \left(\int \left(e^{\frac{p^2+\delta}{T}} - 1\right)^{-1} dp\right)^2. \tag{6.2}$$

Note that

$$T \int \ln\left(1 - e^{\frac{-(p^2+\delta)}{T}}\right) dp \leq -Te^{-\delta/T} \int e^{-p^2/T} dp = -C_0 T^{5/2} e^{-\delta/T}, \tag{6.3}$$

where $C_0 = (2\pi)^{-2} \int_0^\infty \sqrt{s} e^{-s} ds < \infty$ (recall our convention for the measures $dp$ and $ds$ explained above (4.1)). Also

$$\int \gamma_\delta(p) dp = T^{3/2} e^{-\delta/T} \int_0^\infty \frac{(2\pi)^{-2}\sqrt{s}}{e^s - e^{-\delta/T}} ds.$$

Clearly,

$$C_0 \leq \int_0^\infty \frac{(2\pi)^{-2}\sqrt{s}}{e^s - e^{-\delta/T}} ds \leq \int_0^\infty \frac{(2\pi)^{-2}\sqrt{s}}{e^s - 1} ds =: C_1, \tag{6.4}$$

and so

$$C_0 T^{3/2} e^{-\delta/T} \leq \int \gamma_\delta(p) \leq C_1 T^{3/2} e^{-\delta/T}. \tag{6.5}$$

Using (6.3) and (6.4) in (6.2) we obtain

$$\mathcal{F}(\gamma_\delta, 0, 0) \leq -C_0 T^{5/2} e^{-\delta/T} - C_0(\delta + \mu) T^{3/2} e^{-\delta/T} + C_1^2 \widehat{V}(0) T^3 e^{-2\delta/T}.$$

We now choose $\delta = \frac{1}{2} T \ln(T)$. Then $e^{-\delta/T} = T^{-1/2}$, which implies

$$\inf_\gamma \mathcal{F}(\gamma, 0, 0) \leq -\frac{C_0}{2} T^2 \ln T + (C_1^2 \widehat{V}(0) - C_0) T^2 - C_0 \mu T,$$

and we arrive at the desired upper bound (6.1).

*Lower bound.* Any minimizer $(\gamma, \alpha, \rho_0)$ has to satisfy

$$\mathcal{F}(\gamma, 0, 0) \geq \mathcal{F}(\gamma, \alpha, \rho_0),$$

which, using monotonicity of the entropy in $\alpha^2$, the fact that $\gamma + \alpha \geq -1/2$, and our assumption $\rho_0 > 0$, implies that

$$\int \gamma(p) dp \leq \frac{\mu + \frac{1}{2} \int \widehat{V}(p) dp}{\widehat{V}(0)} := A > 0, \tag{6.6}$$

where the constant $A$ is positive and only depends on $\mu$ and $V$. Combining this knowledge with the aforementioned facts in the same way, we obtain

$$\mathcal{F}(\gamma, \alpha, \rho_0) \geq \int p^2 \gamma(p) dp - TS(\gamma, 0) - \mu A - \rho_0 A \widehat{V}(0) + \frac{1}{2} \rho_0^2 \widehat{V}(0).$$

A lower bound for the terms involving $\rho_0$ can be calculated explicitly. Using (6.6) again, we obtain for any $\delta \geq 0$:

$$\mathcal{F}(\gamma, \alpha, \rho_0) \geq \int (p^2 + \delta) \gamma(p) dp - TS(\gamma, 0) - \delta A - \mu A - \frac{1}{2} A^2 \widehat{V}(0).$$

To obtain a lower bound, we now minimize the expression involving $\gamma$, which leads to the bound

$$\mathcal{F}(\gamma, \alpha, \rho_0) \geq T \int \ln\left(1 - e^{\frac{-(p^2+\delta)}{T}}\right) dp - \delta A - \mu A - \frac{1}{2} A^2 \widehat{V}(0).$$

Since

$$\ln\left(1 - e^{\frac{-(p^2+\delta)}{T}}\right) \geq -\frac{1}{e^{\frac{p^2+\delta}{T}} - 1},$$

one has

$$T \int \ln\left(1 - e^{\frac{-(p^2+\delta)}{T}}\right) dp \geq -T \int \frac{dp}{e^{\frac{p^2+\delta}{T}} - 1} \geq -C_1 T^{5/2} e^{-\delta/T},$$

where we use (6.5). Thus, choosing $\delta = \frac{3}{2} T \ln T$ we arrive at

$$\mathcal{F}(\gamma, \alpha, \rho_0) \geq -C_1 T - \frac{3}{2} A T \ln T - \mu A - \frac{1}{2} A^2 \widehat{V}(0),$$

which completes the proof of the lower bound. □

We now prove the existence of a phase transition for the canonical problem.

*Proof of Theorem 9. Step 1.* Let $\rho > 0$ be fixed and let $C_0$ be a constant depending on $V$ and $\rho$ that will be fixed later on. Consider

$$U = \left\{ |p| > \sqrt{2\rho\widehat{V}(0) + C_0(\rho, \widehat{V})} \right\} \subset \mathbb{R}^3.$$

There exists a temperature $T_4$ depending only on $\rho$ and $V$ such that for $T > T_4$, we have

$$\rho < \int_U \frac{1}{e^{2p^2/T} - 1} dp. \tag{6.7}$$

We will prove that (6.7) implies that $\rho_0 = 0$ for the minimizer.

To prove this claim, consider any $(\gamma, \alpha, \rho - \int \gamma)$ with $\int \gamma \leq \rho$. Note that by (6.7) there exists a subset $V \subset U$ with positive measure such that

$$\gamma(p)\big|_V < \frac{1}{e^{2p^2/T} - 1}. \tag{6.8}$$

Recall the functional derivative of the canonical functional in (5.16). Using the fact that the gamma-derivative of the entropy is monotone increasing in $\alpha^2$ in the first step and (3.3) in the second (which defines $C_0$), we obtain

$$\begin{aligned}\frac{\partial \mathcal{F}^{\text{can}}}{\partial \gamma} &\leq p^2 - T\ln\left(\frac{\gamma(p)+1}{\gamma(p)}\right) + (\rho - \rho_\gamma)\,\widehat{V}(p) + \widehat{V} * \gamma(p) - \int \widehat{V}(\gamma + \alpha) \\ &\leq p^2 - T\ln\left(\frac{\gamma(p)+1}{\gamma(p)}\right) + 2\rho\widehat{V}(0) + C_0.\end{aligned}$$

The bound (6.8) implies that on $V \subset U$ we have

$$\frac{\partial \mathcal{F}^{\text{can}}}{\partial \gamma}\Big|_{(\gamma,\alpha)} < 0.$$

In particular, we can lower the energy corresponding to any $\gamma$ with $\int \gamma \leq \rho$ by increasing it on some set of non-zero measure. However, this can only be done up to the point where $\int \gamma = \rho$. We therefore conclude that the minimizer will have to satisfy this, and hence $\rho_0 = 0$, which proves the claim.

*Step 2.* We will now show that all $(\gamma, 0, 0)$ with $\int \gamma = \rho > 0$ have a higher energy than $(0, 0, \rho)$ for $0 \leq T < T_3$, where $T_3 > 0$ is a constant temperature depending on $\rho$ and $V$. Since adding an $\alpha$ can never decrease the energy when $\rho_0 = 0$, this suffices. We have

$$\begin{aligned}\mathcal{F}^{\text{can}}(\gamma, 0, 0) =& \frac{1}{2}\int p^2\gamma(p)dp - TS(\gamma, 0) + \frac{1}{2}\widehat{V}(0)\rho^2 \\ &+ \frac{1}{2}\int p^2\gamma(p)dp + \frac{1}{2}\int \widehat{V}(p-q)\gamma(p)\gamma(q)dpdq \\ &\geq -CT^{5/2} + \frac{1}{2}\widehat{V}(0)\rho^2 + \min\left\{c_1\rho, c_2\rho^2\right\},\end{aligned}$$

where in the last step we used an argument similar to the one given in (5.7). Note that the last term is strictly positive and that it only depends on $\rho$ and $V$.

This can be combined with

$$\mathcal{F}^{\text{can}}(0, 0, \rho) = \frac{1}{2}\widehat{V}(0)\rho^2$$

to give the estimate

$$\mathcal{F}^{\mathrm{can}}(\gamma,0,0)-\mathcal{F}^{\mathrm{can}}(0,0,\rho)\geq\min\left\{c_1\rho,c_2\rho^2\right\}-CT^{5/2}.$$

Since the first term is positive and only depends on $\rho$ and $V$, we see that this implies the existence of a $T_3>0$ as described above. □

What remains to be done is to determine the grand canonical phase diagram from Figure 1. Most of the work has already been done. We will now collect some results and see how this diagram has been obtained.

For $\mu>0$, we have Theorem 8 and Lemma 38. Note that (5.8) determines the lower bound of the region with the lighter shade of blue. The bounds derived in the proof of Theorem 8 determine an upper bound on this region, but it does not go to 0 when $\mu$ does. To get the behaviour shown in Figure 1, we need Theorem 12.

The case $T=0$ and $\mu\leq 0$ has been explained at the beginning of Subsection 5.1. By an argument similar to Lemma 22, we know that $\gamma>0$ for $T>0$. What remains to be shown is that there is no condensation for $T>0$ and $\mu\leq 0$. This follows from the fact that $\rho_0>0$ would imply

$$\begin{aligned}\mathcal{F}(\gamma,\alpha,\rho_0)&>\mathcal{F}(\gamma,0,0)+\rho_0\int\widehat{V}(p)\alpha(p)dp+\frac{1}{2}\int\widehat{V}(p-q)\alpha(q)\alpha(p)dpdq\\&\quad+\frac{1}{2}\widehat{V}(0)\rho_0^2+\widehat{V}(0)\rho_\gamma\rho_0\\&>\mathcal{F}(\gamma,0,0)+\frac{1}{2}\int\widehat{V}(p-q)(\alpha+\rho_0\delta)(p)(\alpha+\rho_0\delta)(q)dpdq\\&\geq\mathcal{F}(\gamma,0,0),\end{aligned}$$

where $\delta$ denotes the Dirac delta distribution. Hence $\rho_0=0$ for $\mu\leq 0$. The conclusions for $\alpha$ follow from Theorem 7.

## Appendix A. Derivation of the functional

A.1. **Bogoliubov trial states.** Let $\mathcal{H}$ be a complex, separable Hilbert space with inner product $\langle\cdot,\cdot\rangle$, which is linear in the second variable and anti-linear in the first, and let $\Gamma_{\mathrm{s}}(\mathcal{H})$ be the bosonic Fock space related to $\mathcal{H}$.

Let $\mathcal{O}$ be the algebra of physical observables of the system, represented by densely-defined self-adjoint operators on $\Gamma_{\mathrm{s}}(\mathcal{H})$ . A *state* $\omega:\mathcal{O}\to\mathbb{C}$ of a quantum system is then identified with a positive semi-definite trace class operator $G$ on $\Gamma_{\mathrm{s}}(\mathcal{H})$ with $\mathrm{Tr}(G)=1$ in the following way:

$$\omega(O)=\mathrm{Tr}(OG)\quad\text{for all bounded}\quad O\in\mathcal{O}. \tag{A.1}$$

The operator $G$ is sometimes called the *density matrix*. The dual space $\mathcal{H}^*$ can be identified with $\mathcal{H}$ by the anti-unitary operator $J:\mathcal{H}\to\mathcal{H}^*$ defined by

$$J(f)(g)=\langle f,g\rangle_{\mathcal{H}},\quad\text{for all}\quad f,g\in\mathcal{H}.$$

If $a^*(f)$ and $a(g)$ are the usual bosonic creation and annihilation operators on $\Gamma_{\mathrm{s}}(\mathcal{H})$ satisfying the canonical commutation relations (CCR)

$$[a(g),a^*(f)]=(g,f),\quad[a^*(g),a^*(f)]=0,\quad[a(g),a(f)]=0\quad\forall f,g\in\mathcal{H},$$

then one can introduce the *field* or *generalized creation* and *annihilation* operators on $\mathcal{H} \oplus \mathcal{H}^*$ by

$$\begin{aligned} A(f \oplus Jg) &= a(f) + a^*(g), \\ A^*(f \oplus Jg) &= a^*(f) + a(g), \quad \forall f, g \in \mathcal{H}. \end{aligned}$$

By defining

$$\mathcal{S} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \text{and} \quad \mathcal{J} = \begin{pmatrix} 0 & J^* \\ J & 0 \end{pmatrix} \tag{A.2}$$

one can express the CCR and conjugate relations in the following way:

$$A^*(F_1) = A(\mathcal{J}F_1), \quad [A(F_1), A^*(F_2)] = \langle F_1, \mathcal{S}F_2 \rangle \quad \text{for all} \quad F_1, F_2 \in \mathcal{H} \oplus \mathcal{H}^*.$$

We can now define the *(generalized) one-particle density matrix* (*1-pdm*) $\Gamma : \mathcal{H} \oplus \mathcal{H}^* \to \mathcal{H} \oplus \mathcal{H}^*$ of a state $\omega$ by

$$\langle F_1, \Gamma F_2 \rangle = \omega(A^*(F_2)A(F_1)) \quad \text{for all} \quad F_1, F_2 \in \mathcal{H} \oplus \mathcal{H}^*.$$

Thus a 1-pdm can be written as

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ J\alpha J & 1 + J\gamma J^* \end{pmatrix}, \tag{A.3}$$

where $\gamma : \mathcal{H} \to \mathcal{H}$ and $\alpha : \mathcal{H}^* \to \mathcal{H}$ are linear operators defined by

$$\langle f, \gamma g \rangle = \omega(a^*(g)a(f)), \quad \langle f, \alpha J g \rangle = \omega(a(g)a(f)) \quad \forall f, g \in \mathcal{H}.$$

The definitions above imply in particular that states with finite particle number expectation are those for which $\gamma$ is trace class.
We shall now recall the notion of *quasi-free states.* For our purpose a quasi-free state $\omega$ will be a state satisfying Wick's Theorem. In particular

$$\omega(a_1^\# a_2^\# a_3^\# a_4^\#) = \omega(a_1^\# a_2^\#)\omega(a_3^\# a_4^\#) + \omega(a_1^\# a_4^\#)\omega(a_2^\# a_3^\#) + \omega(a_1^\# a_3^\#)\omega(a_2^\# a_4^\#),$$

where $a^\#$ is either $a$ or $a^*$. Furthermore, for any $m$ we have

$$\omega(a_1^\# \dots a_{2m+1}^\#) = 0.$$

If one considers a Bose system, one should extend the class of variational states by including so-called *coherent states.* These states are used to describe the condensate fraction (for an explanation see e.g. [29]).

The mathematical implementation of that idea relies on the fact that for every $\phi \in \mathcal{H}$ there exists a unitary operator $\mathbb{U}_\phi : \Gamma_{\rm s}(\mathcal{H}) \to \Gamma_{\rm s}(\mathcal{H})$ such that

$$\mathbb{U}_\phi^* a(f) \mathbb{U}_\phi = a(f) + \langle f, \phi \rangle \quad \forall f \in \mathcal{H}.$$

We may now describe the Bogoliubov variational states. Let $\omega_{\gamma,\alpha}$ be the quasi-free state with the 1-pdm $\Gamma_{\gamma,\alpha}$ and let $\phi \in \mathcal{H}$. The *Bogoliubov variational state* $\omega_{\gamma,\alpha,\phi}$ is defined by

$$\omega_{\gamma,\alpha,\phi}(O) := \omega_{\gamma,\alpha}(\mathbb{U}_\phi^* O \mathbb{U}_\phi) \quad \text{for all} \quad O \in \mathcal{O}. \tag{A.4}$$

A.2. **The Hamiltonian part.** Having introduced Bogoliubov variational states we will now turn to the derivation of the functional. Our model is based on the grand canonical Hamiltonian of the form

$$H = T + U = \sum_p (p^2 - \mu) a_p^* a_p + \frac{1}{2L^3} \sum_{p,q,k} \widehat{V}(k) a_{p+k}^* a_{q-k}^* a_q a_p, \tag{A.5}$$

where the summation is taken over momenta $p, k, q \in \frac{2\pi}{L}\mathbb{Z}^3$. Here $a_p = a(L^{-3/2}e^{ipx})$.

Note that (A.5) is the second quantization (in the plane wave basis) of the translation invariant grand canonical $N$-body Hamiltonian

$$H_N = \sum_{i=1}^{N} -\Delta_i^L + \sum_{i<j} V^L(x_i - x_j)$$

defined on $L^2_{\text{sym}}(\Lambda^N)$, where $\Lambda = [-\frac{L}{2}, \frac{L}{2}]^3$ is the physical space on which we impose periodic boundary conditions. The Laplacian is supposed to have periodic boundary conditions on $\Lambda$. The function $V^L$ is the periodized potential given by

$$V^L(x) = \sum_{n\in\mathbb{Z}^3} V(x + nL).$$

We also have

$$\mathbb{U}_\phi^* a_p \mathbb{U}_\phi = a_p + \langle L^{-3/2} e^{ipx}, \phi(x)\rangle.$$

Bogoliubov's $c$-number substitution ([20]) is then implemented by choosing $\phi(x)$ to be a constant function equal to $\sqrt{\rho_0}$, where, as mentioned in the introduction, $\rho_0 \geq 0$ has the interpretation of being the condensate density. Thus

$$\mathbb{U}_\phi^* a_p \mathbb{U}_\phi = a_p + \delta_{p,0}\sqrt{\rho_0}\sqrt{|\Lambda|}.$$

According to (A.3) we define

$$\gamma(k) := \omega_{\gamma,\alpha}(a_k^* a_k), \qquad \text{and} \qquad \alpha(k) := \omega_{\gamma,\alpha}(a_k a_{-k}).$$

We assume furthermore that our trial states satisfy

$$\omega_{\gamma,\alpha}(a_k a_{-k}) = \omega_{\gamma,\alpha}(a_k^* a_{-k}^*).$$

A straightforward calculation, using the properties of quasi-free states and translation invariance of the system, then implies that

$$\begin{aligned}
\omega_{\gamma,\alpha,\sqrt{\rho_0}}(H) = {} & \sum_p (p^2 - \mu)\gamma(p) - \mu|\Lambda|\rho_0 + \frac{\widehat{V}(0)}{2|\Lambda|} \sum_{p,q} \gamma(p)\gamma(q) \\
& + \frac{1}{2|\Lambda|} \sum_{p,q} \left[ \widehat{V}(p-q) \left( \alpha(p)\alpha(q) + \gamma(p)\gamma(q) \right) \right] \\
& + \frac{\rho_0^2 |\Lambda| \widehat{V}(0)}{2} + \widehat{V}(0)\rho_0 \sum_k \gamma(k) + \rho_0 \sum_k \widehat{V}(k) \left( \gamma(k) + \alpha(k) \right).
\end{aligned}$$

The *thermodynamic free energy* (per volume), $\mathcal{F}$, of a state $\omega$ at temperature $T \geq 0$ and chemical potential $\mu \in \mathbb{R}$ is defined as

$$\mathcal{F}(\omega) = \frac{1}{|\Lambda|} \Big( \omega(H) - TS(\omega) \Big).$$

Taking the informal macroscopic limit $|\Lambda| \to \infty$ and assuming that $\frac{1}{|\Lambda|}\sum_p \to (2\pi)^{-3}\int dp$ we obtain the desired variational expression for the Hamiltonian part of the free energy density.

A.3. **The entropy part.** We now derive the formula for the entropy density in a Bogoliubov trial state in terms of $\gamma, \alpha$, and $\phi$. To do this we will use some basic facts concerning *Bogoliubov transformations* see, e.g. [22].

Given a state $\omega$ with a corresponding density matrix $\mathbb{G}$, its entropy is defined as

$$S(\omega) = -\mathrm{Tr}(\mathbb{G}\ln\mathbb{G}).$$

We only consider Bogoliubov variational states $\omega_{\gamma,\alpha,\phi}$, thus by definitions (A.1) and (A.4) $\mathbb{G} = \mathbb{U}_\phi G \mathbb{U}_\phi^*$ where $G$ is the density matrix corresponding to the quasi-free state $\omega_{\gamma,\alpha}$. Since $\mathbb{U}_\phi$ is unitary we see that

$$\mathrm{Tr}(\mathbb{G}\ln\mathbb{G}) = \mathrm{Tr}(G\ln G)$$

and so

$$S(\omega_{\gamma,\alpha,\phi}) = S(\omega_{\gamma,\alpha}).$$

This means that the coherent transformation, i.e. the condensate, does not change the entropy. Thus, if we want to calculate the entropy of Bogoliubov trial states it is enough to consider quasi-free states. For such a state the density matrix $G$ is unitarily equivalent through a Bogoliubov transformation to an operator of the form

$$\tilde{G} = Z^{-1}\Pi\exp\left[-\sum_{i\in I} e_i a_i^* a_i\right]\Pi, \quad Z = \prod_{i\in I}\frac{1}{1-e^{-e_i}}$$

where $a_i := a(u_i)$ for an orthonormal basis $\{u_i\}$ of the Hilbert space, $I \subseteq \mathbb{N}$, $e_i \geq 0$, and $\Pi$ is the projection onto the subspace $\ker\left[\sum_{i\notin I} a_i^* a_i\right]$. The constant $Z$ (which will be finite) ensures that $\mathrm{Tr}(\tilde{G}) = 1$. The 1-pdm $\tilde{\Gamma}$ of $\tilde{G}$ is easily seen to have $\tilde{\alpha} = 0$ and $\tilde{\gamma}$ diagonal in the basis $\{u_i\}$ with eigenvalues $\lambda_i$ given by

$$(1-\exp(-e_i))^{-1} = 1 + \lambda_i, \quad i \in I,$$

and zero otherwise.

For the state above one can easily calculate the entropy. The Fock space $\Gamma_{\mathrm{s}}(\mathcal{H})$ has the orthonormal basis

$$|\vec{n}\rangle := |n_1, n_2, \ldots\rangle = (n_1! n_2! \ldots)^{-\frac{1}{2}}(a_1^*)^{n_1}(a_2^*)^{n_2}\ldots|0\rangle,$$

where $|0\rangle$ is the Fock vacuum and $n_1, n_2, \ldots \in \mathbb{N}\cup\{0\}$ with only a finite number of $n_j$'s that are positive. We find

$$S(\tilde{G}) = \sum_{i\in I}\ln(1+\lambda_i) + \sum_{j\in I}\sum_{\{\vec{n}\}}\langle\vec{n}|\frac{e_j a_j^* a_j \exp[-e_j a_j^* a_j]}{\prod_{i\in I}(1+\lambda_i)}|\vec{n}\rangle\prod_{i\in I, i\neq j}(1+\lambda_i),$$

which together with

$$\sum_{\{\vec{n}\}}\langle\vec{n}|e_j a_j^* a_j \exp[-e_j a_j^* a_j]|\vec{n}\rangle = \sum_{n_j=0}^{\infty} e_j n_j e^{-e_j n_j} = \frac{e_j e^{-e_j}}{(1-e^{-e_j})^2}$$

and the definition of $e_j$ implies that

$$S(\tilde{G}) = \sum_{i\in I} \ln(1+\lambda_i) - \sum_{j\in I} \lambda_j \ln\left(\frac{\lambda_j}{1+\lambda_j}\right)$$
$$= \sum_{j\in I} \left[(1+\lambda_j)\ln(1+\lambda_j) - \lambda_j \ln \lambda_j\right].$$

It is, however, not immediately possible to find the entropy of $G$ in terms of its 1-pdm $\Gamma$ from this formula. In fact, although $G$ and $\tilde{G}$ are unitarily equivalent, this is not so for $\Gamma$ and $\tilde{\Gamma}$. The relation however is (see [22]) that $\Gamma' = (\Gamma + \frac{1}{2}\mathcal{S})^{1/2}\mathcal{S}(\Gamma + \frac{1}{2}\mathcal{S})^{1/2}$ and $\tilde{\Gamma}' = (\tilde{\Gamma} + \frac{1}{2}\mathcal{S})^{1/2}\mathcal{S}(\tilde{\Gamma} + \frac{1}{2}\mathcal{S})^{1/2}$ are unitarily equivalent. Since we can express the entropy of $\tilde{G}$ as

$$S(\tilde{G}) = -\operatorname{Tr}\left((\tilde{\Gamma}' - \frac{1}{2})\ln|\tilde{\Gamma}' - \frac{1}{2}|\right).$$

We have proved the following result.

**Theorem 39.** *Let $\omega_{\gamma,\alpha}$ be a quasi-free state with 1-pdm $\Gamma$. The entropy of this state is given by*

$$S(\omega_{\gamma,\alpha}) = -\operatorname{Tr}\left((\Gamma' - \frac{1}{2})\ln|\Gamma' - \frac{1}{2}|\right)$$

*where $\Gamma' = (\Gamma + \frac{1}{2}\mathcal{S})^{1/2}\mathcal{S}(\Gamma + \frac{1}{2}\mathcal{S})^{1/2}$.*

In our case

$$\Gamma + \frac{1}{2}\mathcal{S} = \begin{pmatrix} \gamma + \frac{1}{2} & \alpha \\ \alpha & \gamma + \frac{1}{2} \end{pmatrix}.$$

To calculate the eigenvalues of $\Gamma'$ we again use the translation invariance of our system and pass to the Fourier space. In the momentum representation the eigenvalues are given by

$$\eta(p) = \pm\sqrt{(\frac{1}{2} + \gamma(p))^2 - \alpha(p)^2}$$

(note that the eigenvalues of $\Gamma'$ are the same by a similarity transformation as the eigenvalues of $\Gamma\mathcal{S} + \frac{1}{2}$) and we arrive at the desired formula. Note that all terms are well-defined since the condition $\Gamma \geq 0$ implies that

$$\gamma(p) \geq 0 \qquad \text{and} \qquad \gamma(p)(1+\gamma(p)) - \alpha(p)^2 \geq 0.$$

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# Paper II

**The Bogoliubov free energy functional II.
The dilute limit**

# THE BOGOLIUBOV FREE ENERGY FUNCTIONAL II. THE DILUTE LIMIT

MARCIN NAPIÓRKOWSKI, ROBIN REUVERS, AND JAN PHILIP SOLOVEJ

Abstract. We analyse the canonical Bogoliubov free energy functional in three dimensions at low temperatures in the dilute limit. We prove existence of a first-order phase transition and, in the limit $\int V \to 8\pi a$, we determine the critical temperature to be $T_{\rm c} = T_{\rm fc}(1 + 1.49\rho^{1/3}a)$ to leading order. Here, $T_{\rm fc}$ is the critical temperature of the free Bose gas, $\rho$ is the density of the gas and $a$ is the scattering length of the pair-interaction potential $V$. We also prove asymptotic expansions for the free energy. In particular, we recover the Lee–Huang–Yang formula in the limit $\int V \to 8\pi a$.

## Contents



## 1. Introduction

For a *non-interacting*, or *free*, Bose gas with density $\rho$, the textbook argument by Einstein shows that the phase transition to BEC happens at a critical temperature (in units $\hbar = 2m = k_B = 1$)

$$T_{\rm fc} = 4\pi\zeta(3/2)^{-2/3}\rho^{2/3}. \tag{1.1}$$

*Date*: October 31, 2016.

How do interactions between the bosons affect this free critical temperature? A system of particular interest is liquid helium, in which the nuclei interact rather strongly through a potential that can be approximated by a hard-core potential, and one can ask how Einstein's argument and the free critical temperature (1.1) are altered by this potential. Feynman studied this problem with path integrals [11, 12]. Arguing that the potential resulted in an increased effective mass, he predicted that the critical temperature would decrease compared to the free case, which had indeed been observed for liquid helium. He did not make any quantitative predictions.

To make such quantitative predictions, various simplifications were considered. The first one is to replace the interaction potential for liquid helium by a hard-core potential with radius $a > 0$

$$V(x) = \begin{cases} \infty & |x| \leq a \\ 0 & |x| > a \end{cases}. \tag{1.2}$$

To simplify things further, it is common to study a weakly-interacting or dilute gas. For a hard-core potential, the natural length scale is given by the radius $a$. We could compare this length scale to the one defined by the density: $\rho^{-1/3}$, the average distance between the particles. Diluteness now means that the particles meet only rarely, that is, the average distance between the particles is much bigger than the length scale of the potential, or

$$\rho^{1/3} a \ll 1. \tag{1.3}$$

This assumption is not valid for liquid helium, but it is for experiments with trapped dilute cold gases such as [3, 8]. In any case, one can repeat Feynman's question: how is the free critical temperature (1.1) altered by the hard-core interaction?

Lee and Yang were the first to study this [21] in the translation-invariant case. They used pseudopotential methods developed in [19, 22] to conclude that the shift in critical temperature should be proportional to $\rho^{1/3}a$. In the appendix of [21], they solve a simplified system, which gives

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + 1.79(\rho^{1/3}a) + o(\rho^{1/3}a)). \tag{1.4}$$

It is such an approximate expression that we will be looking for in this paper, but for a general class of potentials. To properly define the dilute limit (1.3) without reference to a hard-core potential, we consider a characteristic length scale of the potential that is known as the *scattering length* $a$ (see [23] for a definition). It coincides with the core radius for the hard-core potential.

For general potentials, there has been a lot of debate about whether the linear dependence on $\rho^{1/3}a$ in (1.4) is correct ([16, 17, 18, 32] predict exponents of 1/2, 3/2, 1/2 and 1/2, respectively, where the latter is the only one predicting a decrease in $T_{\mathrm{c}}$ compared to $T_{\mathrm{fc}}$). Nonetheless, (1.4) is still expected to hold true, at least up to the value of the constant 1.79, which we discuss shortly.

It is good to remember that the search for (1.4) for general potentials started from a desire to understand BEC in superfluid helium, but that that particular problem remains intractable to this day. In its stead, the dilute setting has become a well-known and challenging object of study of its own. Indeed, the predicted critical temperature for a dilute gas (1.4) is higher than $T_{\rm fc}$, whereas the critical temperature of liquid helium is lower, which shows that the systems are quite different. Nonetheless, we have little hope of understanding the strongly-interacting case if we cannot even treat this weakly-interacting set-up, justifying the attention this problem has received (see [2] for an overview).

We start from a Hamiltonian for a gas of $N$ bosons that interact via a (periodized) repulsive pair potential $V^l$ in a three-dimensional box $[-l/2, l/2]^3$ with periodic boundary conditions:

$$H_N = \sum_{1\leq i\leq N} -\Delta_i^l + \sum_{1\leq i<j\leq N} V_{ij}^l.$$

The particle density is $\rho = N/l^3$. Assuming the interaction only depends on the distance between the particles, $H_N$ is translation invariant, and we therefore write its second-quantized form in momentum space

$$H = \sum_p p^2 a_p^\dagger a_p + \frac{1}{2l^3} \sum_{p,q,k} \widehat{V}^l(k) a_{p+k}^\dagger a_{q-k}^\dagger a_q a_p. \tag{1.5}$$

Here, only particular $p$ are included in the sum, as determined by the size of the box $l$, but we will consider the thermodynamic limit $l \to \infty$.

To the best of our knowledge, the only rigorous fact known about the critical temperature for the Hamiltonian (1.5) is the upper bound established by Seiringer and Ueltschi using the Feynman–Kac formula [28]. It is not surprising that such results are thin on the ground: it remains impossible to prove BEC in the dilute limit at positive temperature, let alone determine the critical point exactly.

As for approximate models, we already mentioned Lee and Yang's expression (1.4) for the hard-core gas [21]. This expression can only be found in the appendix of their paper, perhaps because Lee and Yang considered their calculation to be physically inaccurate since it predicts a first—rather than the expected second—order phase transition. The fact that (1.4) was hidden in the appendix has presumably led to the widespread misconception that Lee and Yang only predicted a shift linear in $\rho^{1/3}a$, without saying anything about the sign or size of the constant [2, 4, 28, 29]. Even if Lee and Yang themselves did not really trust their result, it fits reasonably well with numerics: Monte Carlo methods [1, 20, 26] suggest that the form (1.4) is correct, but that the numerical value 1.79 should be closer to 1.3.

So how do Lee and Yang approach this problem? They replace the boundary conditions imposed by the hard-core potential by a pseudopotential that should give the right wave function in the physically relevant region where all the particles are at least distance $2a$ from one another [19, 22]. They then assume that only s-wave scattering is important (i.e. the momentum of the particles is low), and show that replacing the potential by

$$8\pi a\delta(\boldsymbol{r})\partial_r r,$$

should yield the correct wave function. For smooth functions, this is simply a multiplication by a delta function, but the derivative does play a role for physical wave functions. All this leads to an excitation spectrum of Bogoliubov form, which can now be used to calculate the shift in the critical temperature (1.4).

Before we explain how this is done, let us point out that this claim in itself has led to some confusion. In a number of articles in which the dilute Bose is treated with field-theoretic methods—e.g. Bijlsma and Stoof [5] and Baym et al. [4], who find (1.4) with constants of 4.7 and 2.9, respectively—it is claimed that mean-field theories such as Bogoliubov's will simply give $T_{\rm c} = T_{\rm fc}$, or, in other words, no shift. One argument [2] goes as follows: a particle with momentum $p$ effectively has the energy

$$\varepsilon(p) \sim \sqrt{p^2(p^2 + 2\widehat{V}(p)\rho)} \approx p^2\sqrt{1 + 2\widehat{V}(0)\rho/p^2} \approx p^2 + \widehat{V}(0)\rho, \qquad (1.6)$$

in which the reader can recognize an approximation to the Bogoliubov dispersion relation [6]. Inserting this 'mean-field' shift of the energy levels into the particle density of the free Bose gas gives

$$\frac{1}{e^{(p^2+\widehat{V}(0)\rho-\mu)/T} - 1} \qquad (1.7)$$

so that the 'critical' $\mu$ is $\widehat{V}(0)\rho$. At this $\mu$, the relation between $T$ and $\rho$ is the same as for the free gas, and so the critical temperature does not change. However, one should be more careful in the comparison with the free gas, and the exact form of the dispersion relation one uses.

In Bogoliubov's analysis, the number of particles $N_0$ in the $p = 0$ state enters via a c-number substitution and plays a crucial role. Dividing by the volume, we obtain a *condensate density* $\rho_0 = N_0/l^3$ that can now be regarded as a parameter. The dispersion relation Lee and Yang derive for the hard-core potential with radius $a$ is

$$\varepsilon(p) \sim \sqrt{p^2(p^2 + 16\pi a\rho_0)}, \qquad (1.8)$$

so, unlike (1.6), this gives a $\rho_0$-dependence. Furthermore, we should not define $\mu$ using the free particle density (1.7), which just happened to be the minimizer of the free energy in that case. Instead, for fixed $\rho$ and $\rho_0$, we should treat the remaining particles with density $\rho - \rho_0$ grand canonically, resulting in a grand canonical partition function that depends on $T$, $\rho$, $\rho_0$ and a chemical potential $\mu$. Recalling that there are only two independent parameters, one should now eliminate $\rho$ by calculating the value it takes at the minimum of the free energy for fixed $T$, $\rho_0$ and $\mu$, and then minimize over all $\rho_0$. The critical $\mu_{\rm c}$ for fixed temperature is the one where the minimizing $\rho_0$ changes from $\rho_0 = 0$ (no BEC) to $\rho_0 > 0$ (BEC). Note that this definition is far more complicated than the naive conclusion $\mu_{\rm c} = \widehat{V}(0)\rho$ above, but it is more correct. That was apparently clear to Lee and Yang, but it seems to have gone out of fashion, resulting in the false belief that the Bogoliubov spectrum does not give a change in the critical temperature.

The treatment of the condensate $\rho_0$ as a separate parameter that defines the critical point is key to our analysis. Another important ingredient is a variational approach introduced by Critchley and Solomon [7]. They evaluate the expectation value of $H - TS - \mu\mathcal{N}$ of a quasi-free state, where $S$ is the von Neumann entropy and $\mathcal{N}$ is the particle number operator, and minimize over all quasi-free states, resulting in an upper bound to the free energy at temperature $T$ and chemical potential $\mu$.

This upper bound is well-motivated. The first supporting argument is that the usual treatment of the Hamiltonian (1.5) with the Bogoliubov approximation [6] reduces it to an operator that is quadratic in the creation and annihilation operators, and that ground and Gibbs states of such operators are quasi-free states. A second is that quasi-free states have successfully served as trial states to establish correct bounds on the ground state energy of Bose gases [10, 15, 31], which is of course the $T = 0$ free energy.

Expressing the expectation value of $H - TS - \mu\mathcal{N}$ for a general quasi-free state does lead to a complicated non-linear functional. Simplifying it somewhat by throwing out certain terms, Critchley and Solomon conclude that the model will reproduce Bogoliubov's conclusions.

In this paper, we consider their functional without the simplifications, and determine whether the minimizers display BEC ($\rho_0 > 0$) or not ($\rho_0 = 0$). This is a variational reformulation of Bogoliubov's and Lee and Yang's approach that is conceptually clear and more accurate, although it has in common with Lee and Yang's approach that the phase transition is of (presumably unphysical) first order.

Our approximation to the critical temperature is

$$T_{\mathrm{c}} = T_{\mathrm{fc}}(1 + 1.49\rho^{1/3}a + o(\rho^{1/3}a)), \tag{1.9}$$

in the limit $\int V = \widehat{V}(0) \to 8\pi a$, and the constant 1.49 is indeed closer to the predicted 1.3 [1, 20, 26] than Lee and Yang's 1.79.

By its construction, this model also gives an upper bound to the free energy at positive temperature, which, for the full Hamiltonian (1.5), was so far only considered by Seiringer [27] and Yin [34]. At $T = 0$, the free energy is simply the ground state energy, which we can compare with the prediction

$$4\pi a\rho^2 + \frac{512}{15}\sqrt{\pi}(\rho a)^{5/2} + o((\rho a)^{5/2})$$

by Lee, Huang and Yang [22]. Our model does reproduce the leading behaviour, but the second order only comes out correctly in the limit $\widehat{V}(0) \to 8\pi a$. A similar result was obtained earlier by Erdös, Schlein and Yau [10], but the exact upper bound has in fact been proved by Yau and Yin [33].

One could ask whether the predicted critical temperature shift (1.9) can actually be measured. For harmonic traps, a linear shift has indeed been measured [9, 14, 30], but it cannot be compared with (1.9) since there is no translation invariance and the effect of the trap, expected to lower rather than raise the critical temperature, is simply too big. Recently, a BEC was also created in a uniform potential [13]. The measurements are not precise enough, however, to measure the shift directly, but even if they were, in this set-up the finite size effects due to the boundedness of the trap are expected to be six times larger than the shift caused by the interaction. In the words of [29], 'we are thus still lacking a direct measurement of the historically most debated [$T_{\rm c}$] shift'.

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## 2. The Bogoliubov free energy functional

This article is the continuation of the previous work [25], in which we derive and analyse the *Bogoliubov free energy functional* that was first introduced by Critchley and Solomon [7]. Let us briefly recall the set-up.

As motivated in the introduction, the functional is obtained from (1.5) by substituting a c-number $\rho_0$ through $a_0 \to a_0 + \sqrt{l^3\rho_0}$ (justified in [24]) and evaluating the expectation value of $H - TS - \mu\mathcal{N}$ of a quasi-free state. Assuming translation invariance and $\langle a_p a_{-p}\rangle = \langle a^\dagger_{-p} a^\dagger_p\rangle$, the two (real-valued) functions $\gamma(p) := \langle a^\dagger_p a_p\rangle \geq 0$ and $\alpha(p) := \langle a_p a_{-p}\rangle$ fully determine this expectation value. Here, $\gamma(p)$ is the *density of particles with momentum p*, and $\alpha$ describes the *pairing in the system.* A non-vanishing $\alpha$ can be interpreted as the presence of off-diagonal long-range order (ODLRO) and the macroscopic coherence related to superfluidity. The c-number $\rho_0 \geq 0$ should be thought of as the *density of the condensate*, so that there is a Bose–Einstein condensate (BEC) if $\rho_0 > 0$. The total particle density is

$$\rho = \rho_0 + (2\pi)^{-3}\int_{\mathbb{R}^3} \gamma(p)dp =: \rho_0 + \rho_\gamma.$$

In the thermodynamic limit, this gives the (grand canonical) Bogoliubov free energy functional

$$\begin{aligned}\mathcal{F}(\gamma,\alpha,\rho_0) = (2\pi)^{-3}&\int_{\mathbb{R}^3} p^2\gamma(p)dp - \mu\rho - TS(\gamma,\alpha) + \frac{\widehat{V}(0)}{2}\rho^2 \\ &+ \rho_0(2\pi)^{-3}\int_{\mathbb{R}^3}\widehat{V}(p)\left(\gamma(p)+\alpha(p)\right)dp. \\ &+ \frac{1}{2}(2\pi)^{-6}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\widehat{V}(p-q)\left(\alpha(p)\alpha(q)+\gamma(p)\gamma(q)\right)dpdq,\end{aligned} \tag{2.1}$$

with entropy

$$\begin{aligned}S(\gamma,\alpha) = \quad &(2\pi)^{-3}\int_{\mathbb{R}^3} s(\gamma(p),\alpha(p))dp \quad = \quad (2\pi)^{-3}\int_{\mathbb{R}^3} s(\beta(p))dp \\ = (2\pi)^{-3}&\int_{\mathbb{R}^3}\left[\left(\beta(p)+\frac{1}{2}\right)\ln\left(\beta(p)+\frac{1}{2}\right) - \left(\beta(p)-\frac{1}{2}\right)\ln\left(\beta(p)-\frac{1}{2}\right)\right]dp,\end{aligned}$$

where

$$\beta(p) := \sqrt{\left(\frac{1}{2}+\gamma(p)\right)^2 - \alpha(p)^2}. \tag{2.2}$$

The functional is defined on the domain $\mathcal{D}$ given by

$$\mathcal{D} = \{(\gamma,\alpha,\rho_0) \mid \gamma \in L^1((1+p^2)dp),\ \gamma \geq 0,\ \alpha(p)^2 \leq \gamma(1+\gamma),\ \rho_0 \geq 0\}.$$

To reiterate, this functional describes the grand canonical free energy of a homogeneous Bose gas at temperature $T \geq 0$ and chemical potential $\mu \in \mathbb{R}$ in the thermodynamic limit.

The goal of the first paper [25] is twofold: to establish the existence of minimizers for the minimization problem

$$F(T,\mu) = \inf_{(\gamma,\alpha,\rho_0)\in\mathcal{D}} \mathcal{F}(\gamma,\alpha,\rho_0), \tag{2.3}$$

and to analyse their structure (in whether $\rho_0 > 0$ or not) for different temperatures and chemical potentials. Keeping in mind that the dilute limit $\rho^{1/3}a \ll 1$ is defined in terms of the density, the canonical counterparts to (2.1) and (2.3) are considered as well: the functional $\mathcal{F}^{\text{can}} = \mathcal{F} + \mu\rho$ at density $\rho \geq 0$ and temperature $T \geq 0$ is given by

$$\begin{aligned}\mathcal{F}^{\text{can}}(\gamma,\alpha,\rho_0) = (2\pi)^{-3}&\int_{\mathbb{R}^3} p^2\gamma(p)dp - TS(\gamma,\alpha) + \frac{1}{2}\widehat{V}(0)\rho^2 \\ &+ (2\pi)^{-3}\rho_0 \int_{\mathbb{R}^3} \widehat{V}(p)\left(\gamma(p)+\alpha(p)\right)dp \\ &+ (2\pi)^{-6}\frac{1}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3} \widehat{V}(p-q)\left(\alpha(p)\alpha(q)+\gamma(p)\gamma(q)\right)dpdq,\end{aligned} \tag{2.4}$$

with $\rho_0 = \rho - \rho_\gamma$. The canonical minimization problem is

$$\begin{aligned}F^{\text{can}}(T,\rho) &= \inf\{\mathcal{F}^{\text{can}}(\gamma,\alpha,\rho_0 = \rho-\rho_\gamma) \mid (\gamma,\alpha,\rho_0=\rho-\rho_\gamma)\in\mathcal{D}\} \\ &= \min\{f(\rho,\rho_0) \mid 0 \leq \rho_0 \leq \rho\},\end{aligned} \tag{2.5}$$

where

$$f(\rho,\rho_0) = \inf\{\mathcal{F}^{\text{can}}(\gamma,\alpha,\rho_0) \mid (\gamma,\alpha,\rho_0)\in\mathcal{D},\ \rho_\gamma = \rho-\rho_0\}.$$

Strictly speaking, this is not really a canonical formulation: it is only the expectation value of the number of particles that we fix. We will nevertheless describe this energy as 'canonical'. The function $F(T,\mu)$ as a function of $\mu$ is the Legendre transform of the function $F^{\text{can}}(T,\rho)$ as a function of $\rho$.

The main results of [25], which we recall in the next section, state that there exist minimizers for both (2.3) and (2.5) and that both models exhibit a BEC phase transition.

## 3. Existence of minimizers and phase transition

The following results, proven in the accompanying paper [25], provide the basis for any further analysis of the Bogoliubov free energy functional.

Throughout this article, we assume that the two-body interaction potential and its Fourier transform

$$\widehat{V}(p) = \int_{\mathbb{R}^3} V(x)e^{-ipx}dx, \qquad V(x) = (2\pi)^{-3}\int_{\mathbb{R}^3} \widehat{V}(p)e^{ipx}dp$$

are radial functions that satisfy

$$V \geq 0, \quad \widehat{V} \geq 0, \quad V \not\equiv 0. \tag{3.1}$$

Moreover, we assume that

$$\widehat{V} \in C^1(\mathbb{R}^3),\ \widehat{V} \in L^1(\mathbb{R}^3),\ \|\widehat{V}\|_\infty < \infty,\ \|\nabla\widehat{V}\|_2 < \infty,\ \|\nabla\widehat{V}\|_\infty < \infty. \tag{3.2}$$

**Theorem 1** (Existence of grand canonical minimizers for $T > 0$)**.** *Let $T > 0$. Assume the interaction potential is a radial function that satisfies* (3.1) *and* (3.2)*. Then there exists a minimizer for the Bogoliubov free energy functional* (2.1) *defined on $\mathcal{D}$.*

It turns out that we need to assume some additional regularity on the interaction potential to prove a similar statement for $T = 0$.

**Theorem 2** (Existence of grand canonical minimizers for $T = 0$)**.** *Assume the interaction potential fulfils the assumptions of Theorem 1. If we assume in addition that $\widehat{V} \in C^3(\mathbb{R}^3)$ and that all derivatives of $\widehat{V}$ up to third order are bounded, then there exists a minimizer for the Bogoliubov free energy functional* (2.1) *defined on $\mathcal{D}$ for $T = 0$.*

We would like to stress that the minimizers need not be unique. In fact, we will see (cf. Remark 38) that there exist combinations of $\mu$ and $T$ for which the problem (2.3) has two minimizers with two different densities.

We have analogous results in the canonical setting.

**Theorem 3** (Existence of canonical minimizers for $T > 0$)**.** *Let $T > 0$. Assume the interaction potential is a radial function that satisfies* (3.1) *and* (3.2)*. Then the variational problem* (2.5) *admits a minimizer.*

**Theorem 4** (Existence of canonical minimizers for $T = 0$)**.** *Assume the interaction potential fulfils the assumptions of Theorem 3. If we assume in addition that $\widehat{V} \in C^3(\mathbb{R}^3)$ and that all derivatives of $\widehat{V}$ up to third order are bounded, then there exists a minimizer for the canonical minimization problem* (2.5) *at $T = 0$.*

Let us now recall the results concerning the existence of phase transitions in our model. Our first result shows that Bose–Einstein Condensation and superfluidity are equivalent in these models.

**Theorem 5** (Equivalence of BEC and superfluidity)**.** *Let $(\gamma, \alpha, \rho_0)$ be a minimizing triple for either* (2.1) *or* (2.4)*. Then*

$$\rho_0 = 0 \Longleftrightarrow \alpha \equiv 0.$$

Thus, there can only be one kind of phase transition, and the next results show that it indeed exists.

**Theorem 6** (Existence of grand canonical phase transition)**.** *Given $\mu > 0$. Then there exist temperatures $0 < T_1 < T_2$ such that a minimizing triple $(\gamma, \alpha, \rho_0)$ of* (2.3) *satisfies*

(1) $\rho_0 = 0$ *for* $T \geq T_2$*;*
(2) $\rho_0 > 0$ *for* $0 \leq T \leq T_1$*.*

**Theorem 7** (Existence of canonical phase transition)**.** *For fixed* $\rho > 0$ *there exist temperatures* $0 < T_3 < T_4$ *such that a minimizing triple* $(\gamma, \alpha, \rho_0)$ *of* (2.5) *satisfies*

(1) $\rho_0 = 0$ *for* $T \geq T_4$*;*
(2) $\rho_0 > 0$ *for* $0 \leq T \leq T_3$*.*

## 4. Main results and sketch of proof

We assume that

$$\rho^{1/3} a \ll 1, \tag{4.1}$$

where $a$, the scattering length of the potential, is defined by

$$4\pi a := \int \Delta w = \frac{1}{2} \int V w,$$

and $w$ satisfies

$$-\Delta w + \frac{1}{2} V w = 0 \tag{4.2}$$

in the sense of distributions with $w(x) \to 1$ as $|x| \to \infty$. The quantity $8\pi a$ is often replaced by $\int V = \widehat{V}(0)$, which is its first-order Born approximation. In fact, $\widehat{V}(0) > 8\pi a$ (see [23, Appendix C] for more details). We quantify this discrepancy with the parameter $\nu = \widehat{V}(0)/a$, so that $\nu > 8\pi$. The limit $\nu \to 8\pi$, i.e. $\widehat{V}(0) \to 8\pi a$, is of special interest.

For the proofs, it will sometimes be useful to consider the region $T \leq D\rho^{2/3}$ with $D > 1$ fixed separately, in which case we can rewrite the second condition in (4.1) as

$$\sqrt{T} a \leq \sqrt{D} \rho^{1/3} a \ll 1. \tag{4.3}$$

In particular, since the thermal wavelength $\Lambda \sim \sqrt{T}^{-1}$, the condition (4.3) implies that $a/\Lambda \ll 1$. Furthermore, we define a constant $C$ by

$$\int \widehat{V} \leq C a^{-2} \qquad \text{and} \qquad \|\partial^n \widehat{V}\|_\infty \leq C a^{n+1} \text{ for } 0 \leq n \leq 3, \tag{4.4}$$

where $\partial^n$ is shorthand for all $n$-th order partial derivatives. With this definition, our estimates depend only on $C$ and not on $a$. Throughout the paper, we will also use $C$ to denote any unspecified positive constant.

### 4.1. The critical temperature.

**The critical temperature.** The following theorems contain information about the critical temperature of the phase transition in the dilute limit. Note that $T_{\text{fc}} = c_0 \rho^{2/3}$ is the critical temperature of the free Bose gas, and $\rho_{\text{fc}} = (T/c_0)^{3/2}$ its corresponding critical density.

**Theorem 8** (Canonical critical temperature)**.** *There is a monotone increasing function* $h_1 : (8\pi, \infty) \to \mathbb{R}$ *with* $h_1(\nu) \geq \lim_{\nu \to 8\pi} h_1(\nu) = 1.49$ *such that for any minimizing triple* $(\gamma, \alpha, \rho_0)$ *of* (2.5) *at temperature* $T$ *and density* $\rho$*:*

(1) $\rho_0 \neq 0$ *if* $T < T_{\text{fc}} \left(1 + h_1(\nu)\rho^{1/3} a + o(\rho^{1/3} a)\right)$
(2) $\rho_0 = 0$ *if* $T > T_{\text{fc}} \left(1 + h_1(\nu)\rho^{1/3} a + o(\rho^{1/3} a)\right)$.

**Theorem 9** (Grand-canonical critical temperature)**.** *There is a function* $h_2 : (8\pi, \infty) \to \mathbb{R}$ *with* $\lim_{\nu\to 8\pi} h_2(\nu) = 0.44$ *such that for any minimizing triple* $(\gamma, \alpha, \rho_0)$ *of* (2.3) *at temperature* $T$ *and chemical potential* $\mu$*:*

(1) $\rho_0 \neq 0$ *if* $T < \left(\frac{\sqrt{\pi}}{2\zeta(3/2)}\frac{8\pi}{\nu}\right)^{2/3}\left(\frac{\mu}{a}\right)^{2/3} + h_2(\nu)\mu + o(\mu)$

(2) $\rho_0 = 0$ *if* $T > \left(\frac{\sqrt{\pi}}{2\zeta(3/2)}\frac{8\pi}{\nu}\right)^{2/3}\left(\frac{\mu}{a}\right)^{2/3} + h_2(\nu)\mu + o(\mu)$.

4.2. **Free energy expansion.** The second main result of this paper provides an expansion of the free energy (2.5) in the dilute limit. We first define the integrals that play a central role in our analysis:

$$\begin{aligned}
I_1(d,\sigma,\theta) &= (2\pi)^{-3}\int\Big[\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma} \\
&\qquad\qquad - (p^2+d+(1+\theta)\sigma) + \frac{((1+\theta)\sigma)^2}{2p^2}\Big]dp \\
I_2(d,\sigma,\theta,s) &= (2\pi)^{-3}\int \ln\left(1-e^{-\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2}}\right)dp \\
I_3(d,\sigma,\theta) &= (2\pi)^{-3}\int\left(\frac{p^2+d+(1+\theta)\sigma}{\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma}}-1\right)dp \\
I_4(d,\sigma,\theta,s) &= (2\pi)^{-3}\int\left(e^{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2}}-1\right)^{-1} \\
&\qquad\qquad \times\frac{p^2+ds^2+(1+\theta)\sigma s^2}{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2}}dp.
\end{aligned} \tag{4.5}$$

We will consider $d, \sigma, s \geq 0$, and $-1 \leq \theta \leq 0$. For the following theorems, it suffices to set $\theta = 0$ and $\sigma = 8\pi$. The general form will, however, be needed to study the critical temperature.

**Theorem 10** (Canonical free energy expansion)**.** *Assume that* $T$ *and* $\rho$ *satisfy the conditions* (4.1) *and* (4.3)*. We then have the following expressions for the canonical free energy* (2.5)*.*

(1) *For* $T > T_{\mathrm{fc}}\left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$*, the free energy is*

$$F^{\mathrm{can}}(T,\rho) = F_0(T,\rho) + \widehat{V}(0)\rho^2 + O((\rho a)^{5/2}),$$

*and we have* $\rho_\gamma = \rho$*,* $\rho_0 = 0$ *for the minimizer. Here* $F_0(T,\rho)$ *is the free energy of the non-interacting gas (cf.* (5.20)*).*

(2) *For* $T < T_{\mathrm{fc}}\left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$*, there exists a universal constant* $d_0 > 0$ *such that the free energy is*

$$\begin{aligned}
F^{\mathrm{can}}(T,\rho) = \inf_{0\leq d\leq d_0}&\Big[\frac{1}{2}(\rho a)^{5/2}I_1(d,8\pi,0) + T^{5/2}I_2(d,8\pi,0,\sqrt{\rho_0(d)a/T}) \\
&- d\rho_0(d)a(\rho-\rho_0(d)) \\
&+ \widehat{V}(0)\rho^2 - 8\pi a\rho_0(d)\rho + \rho_0(d)^2(12\pi a - \widehat{V}(0))\Big] \\
&+ o\left(T(\rho a)^{3/2} + (\rho a)^{5/2}\right),
\end{aligned}$$

*where*

$$\rho_0(d) := \rho - \frac{1}{2}(\rho a)^{3/2}I_3(d,8\pi,0) - T^{3/2}I_4(d,8\pi,0,\sqrt{(\rho-\rho_{\mathrm{fc}})a/T}).$$

In fact, we will obtain a more precise energy expansion in the region around the critical temperature.

The expression for the free energy above involves integrals and a minimization problem in the parameter $d$. If we also assume that $\rho a/T \ll 1$, we can simplify the result, as the following theorem shows.

**Theorem 11** (The canonical free energy for $\rho a/T \ll 1$)**.** *Let $\Delta\rho = \rho - \rho_{\mathrm{fc}}$. For $\rho a/T \ll 1$ and $T < T_{\mathrm{fc}}\left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$, the canonical free energy is given by*

$$\begin{aligned} F^{\mathrm{can}}(T,\rho) &= T^{5/2} f_{\min} + 4\pi a\rho^2 + (\nu - 4\pi)a\rho_{\mathrm{fc}}(2\rho - \rho_{\mathrm{fc}}) \\ &\quad + \left(\frac{\Delta\rho a}{T}\right)^{3/2}\left(-\frac{1}{3\sqrt{2}\pi}\right)\left(\nu^{3/2} + (\nu - 8\pi)^{3/2}\right)T^{5/2} \\ &\quad + o(T(\rho a)^{3/2}). \end{aligned}$$

In the case $\rho a/T \gg 1$, we can also simplify the expression in the second point of Theorem 10: the contribution from the integrals $I_2$ and $I_4$ can be neglected in the minimization problem.

**Corollary 12** (The canonical energy for $\rho a/T \gg 1$ )**.** *For $\rho a/T \gg 1$ and $T < T_{\mathrm{fc}}\left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$, the canonical free energy can be described in terms of a function $g : (8\pi, \infty) \to \mathbb{R}$ as*

$$F^{\mathrm{can}}(T,\rho) = 4\pi a\rho^2 + g(\nu)(\rho a)^{5/2} + o\left((\rho a)^{5/2}\right),$$

*with $g(\nu) \to \frac{512}{15}\sqrt{\pi}$ as $\nu \to 8\pi$. The latter result is known as the Lee–Huang–Yang formula.*

Before we proceed to the proof of these theorems, let us sketch the main ideas used in the paper.

4.3. **Set-up of the paper.** Since the Euler–Lagrange equations of the free energy functional involve the convolutions $\widehat{V} * \gamma$ and $\widehat{V} * \alpha$, it is very hard to analyse them quantitatively. Even with a Fourier transform, they cannot be solved. The main idea is to replace the non-local terms in the functional by local ones, such that we end up with a simplified functional that can be minimized explicitly, that is,

$$\inf_{\substack{(\gamma,\alpha,\rho_0) \\ \rho_0 + \rho_\gamma = \rho}} \mathcal{F}^{\mathrm{can}} \approx \inf_{\substack{(\gamma,\alpha,\rho_0) \\ \rho_0 + \rho_\gamma = \rho}} \mathcal{F}^{\mathrm{sim}} = \inf_{0 \le \rho_0 \le \rho}\left[\inf_{\substack{(\gamma,\alpha) \\ \rho_\gamma = \rho - \rho_0}} \mathcal{F}^{\mathrm{sim}}\right]$$

where the final minimizations can be done explicitly.

The approximation involves several steps. First, we replace the convolution term involving $\gamma$ with $\widehat{V}(0)\rho_\gamma^2$. We expect that the particles interact weakly in the dilute limit and it seems reasonable to assume that the system will behave like a free Bose gas to leading order. We therefore expect that the minimizing $\gamma$ is concentrated on a ball of radius $\sqrt{T}$. By our assumptions (4.4), $\widehat{V}(p)$ is approximately $\widehat{V}(0)$ on a ball of radius $a^{-1} \gg \sqrt{T}$ (in the region around the critical temperature), justifying the replacement.

Second, by introducing a trial function $\alpha_0$, we rewrite the convolution terms involving $\alpha$. This trial function will be expressed in terms of $\widehat{Vw}$, where $w$ is the solution to the scattering equation. Finally, we will also substitute $\widehat{V}$ by $\widehat{Vw}$ in the terms that are linear in $\gamma$ at the cost of a small error. All this will be done in Subsection 5.1, with Lemma 13 specifying the error terms exactly.

We then minimize the simplified functional. We split the minimization in two steps: first one over $\gamma$ and $\alpha$ with the constraint that $\rho_0 + \rho_\gamma = \rho$, followed by a minimization over $0 \leq \rho_0 \leq \rho$. The first step will be carried out in Subsection 5.2, and it will lead to a useful class of minimizers $(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta})$. To prepare for the final minimization over $\rho_0$, we will establish further properties of these functions in Subsection 5.6.

In order to prove that this provides a good approximation, we will need to know that the error terms are small for both the minimizer of the full functional and the minimizer of the simplified functional. For the full functional, this is shown in Subsections 5.3 and 5.4 along with several other useful a priori estimates.

In Subsection 5.7, we will analyse the energy in the region $|\rho - \rho_{\mathrm{fc}}| \leq C\rho(\rho^{1/3}a)$, since the a priori result of Subsection 5.5 shows that this is where the phase transition occurs. This leads to the calculation of the critical temperature and the proof of Theorems 8 and 9.

Subsection 5.8 contains the proof of Theorems 10 and 11.

## 5. Proof of the main results

5.1. **Derivation of the simplified functional.** The following simplified functional will serve as an approximation to the canonical free energy functional (2.4):

$$\begin{aligned}
\mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,\rho_0) = (2\pi)^{-3} &\int \left(p^2 + (\rho_0 + t_0)\widehat{Vw}(p)\right)\gamma(p)dp \\
&+ (2\pi)^{-3}\int (\rho_0 + t_0)\widehat{Vw}(p)\alpha(p)dp - TS(\gamma,\alpha) \\
&+ \frac{1}{4}(2\pi)^{-3}(\rho_0+t_0)^2\int \frac{\widehat{Vw}(p)^2}{p^2}dp \\
&+ \widehat{V}(0)\rho^2 + (12\pi a - \widehat{V}(0))\rho_0^2 - 8\pi a\rho\rho_0 \\
&- 4\pi a t_0^2 - 8\pi a t_0(\rho - \rho_0).
\end{aligned} \tag{5.1}$$

Here, $w$ satisfies the scattering equation (4.2), and $t_0$ is a parameter that could in principle be chosen to depend on $\rho$ and $\rho_0$. This will turn out to be necessary for the proof of Theorems 8 and 9 in Subsection 5.7, and we will state a specific choice for $t_0$ at the start of this subsection. For the proof of Theorems 10 and 11 in Subsection 5.8 it will, however, suffice to set $t_0 = 0$. Before we make a choice for $t_0$, we will work with the general assumption

$$-\rho_0 \leq t_0 \leq 0. \tag{5.2}$$

Note that $\mathcal{F}^{\mathrm{sim}}$ consist of terms that are both linear and local in $\gamma$ and $\alpha$ (aside from the entropy), and it will therefore be much easier to handle than the full $\mathcal{F}^{\mathrm{can}}$.

As shown in Lemma 13, the difference between $\mathcal{F}^{\text{sim}}$ and $\mathcal{F}^{\text{can}}$ can be expressed in terms of

$$\begin{aligned}
E_1(\gamma,\alpha,\rho_0) &:= (2\pi)^{-6}\frac{1}{2}\iint(\alpha-\alpha_0)(p)\widehat{V}(p-q)(\alpha-\alpha_0)(q)dpdq \\
E_2(\gamma,\alpha,\rho_0) &:= \left|(2\pi)^{-3}\rho_0\int\gamma(p)\widehat{V}(p)dp-\widehat{V}(0)\rho_0\rho_\gamma\right| \\
E_3(\gamma,\alpha,\rho_0) &:= \left|(2\pi)^{-3}\rho_0\int\gamma(p)\widehat{Vw}(p)dp-\widehat{Vw}(0)\rho_0\rho_\gamma\right| \\
E_4(\gamma,\alpha,\rho_0) &:= \left|(2\pi)^{-6}\frac{1}{2}\iint\gamma(p)\widehat{V}(p-q)\gamma(q)dpdq-\frac{1}{2}\widehat{V}(0)\rho_\gamma^2\right|.
\end{aligned} \tag{5.3}$$

Here, the function $\alpha_0$ is chosen to be

$$\alpha_0 := (\rho_0+t_0)\widehat{w}-(2\pi)^3\rho_0\delta_0 = (2\pi)^3 t_0\delta_0-\frac{\rho_0+t_0}{2}\frac{\widehat{Vw}(p)}{p^2}, \tag{5.4}$$

where we have used the Fourier transform of the scattering equation (4.2), taking into account the boundary condition:

$$\widehat{w} = (2\pi)^3\delta_0-\frac{1}{2}\frac{\widehat{Vw}(p)}{p^2}. \tag{5.5}$$

When a more precise error is required, we will consider

$$\begin{aligned}
E_5(\gamma,\alpha,\rho_0) := \Big|(2\pi)^{-6}\frac{1}{2}\iint & \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq \\
&-\frac{1}{2}\widehat{V}(0)\rho_\gamma^2-\frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4\Big|.
\end{aligned} \tag{5.6}$$

Note that the additional term in $E_5$ compared to $E_4$ is independent of $(\gamma,\alpha,\rho_0)$ and including it in the simplified functional will therefore not affect the minimizer (see Corollary 14).

The function $\widehat{Vw}$ appears in our definition of $\alpha_0$. It will turn out to be convenient to gather some of its properties before we prove the main result of this section. First of all, $w\geq 0$, which implies that $Vw\geq 0$, and so

$$|\widehat{Vw}(p)|\leq\widehat{Vw}(0)=8\pi a.$$

From (5.5), we obtain

$$\int Vw^2 = 8\pi a-\frac{1}{2}(2\pi)^{-3}\int\widehat{Vw}(p)^2|p|^{-2}dp, \tag{5.7}$$

and hence the integral on the left-hand side is bounded by $Ca$. This implies

$$\int|\widehat{Vw}|^2=\int|Vw|^2\leq\|V\|_\infty\int Vw^2\leq\frac{C}{a},$$

where we have used our assumptions (4.4). Using the above conclusions, we now estimate

$$\begin{aligned}
\left\|\frac{\widehat{Vw}}{p^2}\right\|_1 &\leq\int_{|p|\leq a^{-1}}\frac{|\widehat{Vw}|}{p^2}dp+\int_{|p|>a^{-1}}\frac{|\widehat{Vw}|}{p^2}dp \\
&\leq C+\left(\int_{|p|>a^{-1}}|\widehat{Vw}|^2dp\right)^{1/2}\left(\int_{|p|>a^{-1}}\frac{1}{p^4}dp\right)^{1/2}\leq C,
\end{aligned}$$

where it is important that the estimate is independent of $a$. Applying (5.5) again, we have

$$\widehat{Vw} = \widehat{V} - \frac{\widehat{Vw}}{2p^2} * \widehat{V}.$$

By our assumptions (4.4) we have for $0 \leq n \leq 3$:

$$\|\partial^n \widehat{Vw}\|_\infty \leq \|\partial^n \widehat{V}\|_\infty \left(1 + \left\|\frac{\widehat{Vw}}{2p^2}\right\|_1\right) \leq Ca^{n+1}. \tag{5.8}$$

We can therefore estimate derivatives of $\widehat{Vw}$ in the same way as those of $\widehat{V}$, and we will use this in the subsections below.

The main result of this subsection is the following lemma, which compares the simplified and canonical free energy functionals. Its message is that, given that the error terms are small for the minimizers of both the simplified and the full functional, it suffices to analyse the simplified functional.

**Lemma 13.** *For any triple $(\gamma, \alpha, \rho_0)$ we have*

$$\begin{aligned}-\Big(E_2 + E_3 + E_4\Big)(\gamma, \alpha, \rho_0) \leq \mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma, \alpha, \rho_0)& \\ \leq \Big(E_1 + E_2 + E_3 + E_4\Big)(\gamma, \alpha, \rho_0).&\end{aligned}$$

*Proof.* We have

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma, \alpha, \rho_0) &= (2\pi)^{-3}\rho_0 \int \Big(\widehat{V}(p) - \widehat{Vw}(p)\Big)(\gamma(p) + \alpha(p))dp \\ &- (2\pi)^{-3} t_0 \int \widehat{Vw}(p)(\gamma(p) + \alpha(p))dp + \frac{1}{2}\widehat{V}(0)\rho_\gamma^2 - \frac{1}{2}\widehat{V}(0)\rho^2 \\ &+ \frac{1}{2}(2\pi)^{-6} \iint \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \frac{1}{2}\widehat{V}(0)\rho_\gamma^2 \\ &- \frac{1}{4}(2\pi)^{-3}(\rho_0 + t_0)^2 \int \frac{\widehat{Vw}(p)^2}{p^2} dp - (12\pi a - \widehat{V}(0))\rho_0^2 \\ &+ 8\pi a\rho\rho_0 + 4\pi a t_0^2 + 8\pi a t_0(\rho - \rho_0) + E_1(\gamma, \alpha, \rho_0) \\ &+ (2\pi)^{-6} \int \alpha(p)(\widehat{V} * \alpha_0)(p)dp - \frac{1}{2}(2\pi)^{-6} \int \alpha_0(p)(\widehat{V} * \alpha_0)(p)dp.\end{aligned} \tag{5.9}$$

We start by dealing with the last two terms in (5.9). First we have

$$(2\pi)^{-3}\widehat{V} * \alpha_0(p) = (\rho_0 + t_0)\widehat{Vw}(p) - \rho_0\widehat{V}(p),$$

which follows immediately from the definition (5.4). This means that the first term in the last line of (5.9) cancels the $\alpha$-terms in the first two lines of (5.9). We thus have

$$
\begin{aligned}
\mathcal{F}^{\text{can}}(\gamma,\alpha,\rho_0)-\mathcal{F}^{\text{sim}}(\gamma,\alpha,\rho_0) &= (2\pi)^{-3}\rho_0\int\left(\widehat{V}(p)-\widehat{Vw}(p)\right)\gamma(p)dp\\
&-(2\pi)^{-3}t_0\int\widehat{Vw}(p)\gamma(p)dp+\frac{1}{2}\widehat{V}(0)\rho_\gamma^2-\frac{1}{2}\widehat{V}(0)\rho^2\\
&+\frac{1}{2}(2\pi)^{-6}\iint\gamma(p)\widehat{V}(p-q)\gamma(q)dpdq-\frac{1}{2}\widehat{V}(0)\rho_\gamma^2\\
&-\frac{1}{4}(2\pi)^{-3}(\rho_0+t_0)^2\int\frac{\widehat{Vw}(p)^2}{p^2}dp-(12\pi a-\widehat{V}(0))\rho_0^2\\
&+8\pi a\rho\rho_0+4\pi a t_0^2+8\pi a t_0(\rho-\rho_0)+E_1(\gamma,\alpha,\rho_0)\\
&-\frac{1}{2}(2\pi)^{-6}\int\alpha_0(p)(\widehat{V}*\alpha_0)(p)dp.
\end{aligned}
\tag{5.10}
$$

We now deal with the last term in the above equation. Using (5.4), we have

$$
\begin{aligned}
\int\alpha_0(\widehat{V}*\alpha_0) &= \iint\frac{(\rho_0+t_0)\widehat{Vw}(p)}{2p^2}\widehat{V}(p-q)\frac{(\rho_0+t_0)\widehat{Vw}(q)}{2q^2}dpdq\\
&\quad+(2\pi)^6t_0^2\widehat{V}(0)-2t_0(2\pi)^3\int\frac{(\rho_0+t_0)\widehat{Vw}(p)\widehat{V}(p)}{2p^2}dp.
\end{aligned}
\tag{5.11}
$$

Note that

$$
\frac{1}{2}\int Vw^2=\int Vw-\frac{1}{2}\int V+\frac{1}{2}\int V(1-w)^2=8\pi a-\frac{1}{2}\int V+\frac{1}{2}\int V(1-w)^2,
$$

so that

$$
\begin{aligned}
&(2\pi)^{-6}\frac{1}{2}\iint\widehat{(1-w)}(p)\widehat{V}(p-q)\widehat{(1-w)}(q)dpdq\\
&\qquad=\frac{1}{2}\int V-4\pi a-\frac{1}{4}(2\pi)^{-3}\int\widehat{Vw}(p)^2|p|^{-2}dp.
\end{aligned}
\tag{5.12}
$$

These identities together with (5.7) allow us to compute the terms in (5.11). By (5.5), we have

$$
\frac{\widehat{Vw}(p)}{2p^2}=\widehat{(1-w)}(p),
$$

so that it follows from (5.12) that

$$
\begin{aligned}
&\frac{1}{2}(2\pi)^{-6}\iint\frac{(\rho_0+t_0)\widehat{Vw}(p)}{2p^2}\widehat{V}(p-q)\frac{(\rho_0+t_0)\widehat{Vw}(q)}{2q^2}dpdq=\\
&=\frac{1}{2}(\rho_0+t_0)^2\widehat{V}(0)-4\pi a(\rho_0+t_0)^2-\frac{1}{4}(2\pi)^{-3}(\rho_0+t_0)^2\int\widehat{Vw}(p)^2|p|^{-2}dp.
\end{aligned}
$$

Furthermore,

$$
\int\frac{\widehat{Vw}(p)\widehat{V}(p)}{2p^2}=\int\widehat{(1-w)}\widehat{V}=(2\pi)^3\int V(1-w)=(2\pi)^3(\widehat{V}(0)-8\pi a).
$$

Collecting all terms we obtain

$$\begin{aligned}\frac{1}{2}(2\pi)^{-6}\int\alpha_0(\widehat{V}*\alpha_0) &= \frac{1}{2}(\rho_0+t_0)^2\widehat{V}(0) - \frac{(\rho_0+t_0)^2}{4(2\pi)^3}\int\frac{\widehat{Vw}(p)^2}{p^2}dp \\ &\quad - 4\pi a(\rho_0+t_0)^2 - t_0(t_0+\rho_0)(\widehat{V}(0)-8\pi a) + \frac{1}{2}t_0^2\widehat{V}(0) \\ &= \frac{1}{2}(\widehat{V}(0)-8\pi a)\rho_0^2 + 4\pi a t_0^2 - \frac{(\rho_0+t_0)^2}{4(2\pi)^3}\int\frac{\widehat{Vw}(p)^2}{p^2}dp,\end{aligned} \tag{5.13}$$

and inserting (5.13) into (5.10) gives

$$\begin{aligned}\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) - \mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,\rho_0) &= (2\pi)^{-3}\rho_0\int\widehat{V}(p)\gamma(p)dp - \widehat{V}(0)\rho_0\rho_\gamma \\ &\quad - (2\pi)^{-3}(\rho_0+t_0)\int\widehat{Vw}(p)\gamma(p)dp + (\rho_0+t_0)8\pi a\rho_\gamma \\ &\quad + \frac{1}{2}(2\pi)^{-6}\iint\gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \frac{1}{2}\widehat{V}(0)\rho_\gamma^2 \\ &\quad + E_1(\gamma,\alpha,\rho_0).\end{aligned} \tag{5.14}$$

Here, we added and subtracted $\widehat{V}(0)\rho_0\rho_\gamma$ and $8\pi a\rho_\gamma(\rho_0+t_0)$ and used that $\widehat{Vw}(0) = 8\pi a$. Using the definitions (5.3), our assumption (5.2), and the fact that $E_1 \geq 0$ we arrive at the desired result. □

**Corollary 14.** *For any triple $(\gamma,\alpha,\rho_0)$ we have*

$$\begin{aligned}&-\Big(E_2+E_3+E_5\Big)(\gamma,\alpha,\rho_0) \\ &\qquad \leq \left(\mathcal{F}^{\mathrm{can}}-\mathcal{F}^{\mathrm{sim}}\right)(\gamma,\alpha,\rho_0) - \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4 \\ &\qquad \leq \Big(E_1+E_2+E_3+E_5\Big)(\gamma,\alpha,\rho_0).\end{aligned}$$

5.2. **Minimization of the simplified functional in $\gamma$ and $\alpha$.** We will now find the minimizers of the simplified functional (5.1). We note that the minimization problem can be rewritten as

$$\begin{aligned}\inf_{(\gamma,\alpha,\rho_0),\ \rho_\gamma+\rho_0=\rho}\mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,\rho_0) &= \inf_{0\leq\rho_0\leq\rho}\Big[\inf_{(\gamma,\alpha),\ \rho_\gamma=\rho-\rho_0}\mathcal{F}^{\mathrm{s}}(\gamma,\alpha,\rho_0) \\ &\quad + \widehat{V}(0)\rho^2 + (12\pi a-\widehat{V}(0))\rho_0^2 - 8\pi a\rho\rho_0 - 4\pi a t_0^2 - 8\pi a t_0(\rho-\rho_0)\Big],\end{aligned}$$

with

$$\begin{aligned}\mathcal{F}^{\mathrm{s}}(\gamma,\alpha,\rho_0) &= (2\pi)^{-3}\int(p^2+(\rho_0+t_0)\widehat{Vw}(p))\gamma(p)dp \\ &\quad + (2\pi)^{-3}(\rho_0+t_0)\int\widehat{Vw}(p)\alpha(p)dp - TS(\gamma,\alpha) \\ &\quad + \frac{1}{4}(2\pi)^{-3}(\rho_0+t_0)^2\int\frac{\widehat{Vw}(p)^2}{p^2}dp.\end{aligned} \tag{5.15}$$

This suggests that we first focus on the minimization problem

$$\inf_{(\gamma,\alpha),\ \rho_\gamma=\rho-\rho_0}\mathcal{F}^{\mathrm{s}}(\gamma,\alpha,\rho_0).$$

Since $\mathcal{F}^{\mathrm{s}}$ is convex in $\gamma$ and $\alpha$, we can enforce the constraint $\rho_\gamma = \rho - \rho_0$ using a Lagrange multiplier $\delta$. Recall that

$$\beta(p) = \sqrt{\left(\frac{1}{2} + \gamma(p)\right)^2 - \alpha(p)^2},$$

and define

$$\begin{aligned} G(p) &= T^{-1}\sqrt{(p^2 + \delta + (\rho_0 + t_0)\widehat{Vw}(p))^2 - ((\rho_0 + t_0)\widehat{Vw}(p))^2} \\ &= T^{-1}\sqrt{(p^2 + \delta)^2 + 2(p^2 + \delta)(\rho_0 + t_0)\widehat{Vw}(p)}. \end{aligned}$$

The following result states the minimizers of the minimization problem for $\delta \geq 0$.

**Lemma 15** (Simplified functional solution)**.** *Let $\delta \geq 0$, $\rho_0 \geq 0$ and $-\rho_0 \leq t_0 \leq 0$. The minimizer of*

$$\inf_{(\gamma,\alpha)} \left[\mathcal{F}^{\mathrm{s}}(\gamma, \alpha, \rho_0) + \delta \int \gamma\right]$$

*is given by*

$$\begin{aligned} \gamma^{\rho_0,\delta} &= \frac{\beta}{TG}(p^2 + \delta + (\rho_0 + t_0)\widehat{Vw}(p)) - \frac{1}{2} \\ \alpha^{\rho_0,\delta} &= -\frac{\beta}{TG}(\rho_0 + t_0)\widehat{Vw}(p), \end{aligned}$$

*with $\beta$ and $G$ as above, and the minimum is*

$$\begin{aligned} &\mathcal{F}^{\mathrm{s}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) + \delta \int \gamma^{\rho_0,\delta} \\ &= (2\pi)^{-3} T \int \ln(1 - e^{-G(p)})dp \\ &\quad + (2\pi)^{-3}\frac{1}{2} \int \Big[\sqrt{(p^2 + \delta)^2 + 2(p^2 + \delta)(\rho_0 + t_0)\widehat{Vw}(p)} \\ &\qquad - (p^2 + \delta + (\rho_0 + t_0)\widehat{Vw}(p)) + \frac{1}{2}(\rho_0 + t_0)^2\frac{\widehat{Vw}(p)^2}{p^2}\Big]dp. \end{aligned}$$

*Proof.* Since

$$s'(\beta) = \ln\left(\frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}\right),$$

we find the the Euler–Lagrange equations to be

$$\begin{aligned} p^2 + \delta + (\rho_0 + t_0)\widehat{Vw}(p) &= T \ln\left(\frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}\right)\frac{\gamma(p) + \frac{1}{2}}{\beta(p)} \\ (\rho_0 + t_0)\widehat{Vw}(p) &= -T \ln\left(\frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}\right)\frac{\alpha(p)}{\beta(p)}. \end{aligned} \tag{5.16}$$

Squaring and subtracting both equations and using (2.2) we obtain

$$\ln\left(\frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}}\right) = G(p), \quad \beta(p) = \left(e^{G(p)} - 1\right)^{-1} + \frac{1}{2}. \tag{5.17}$$

One may be concerned about the square root in the definition of $G$. However, using $\widehat{Vw}(0) = 8\pi a$, $\widehat{Vw}'(0) = 0$ and $\|\widehat{Vw}''\|_\infty \leq Ca^3$, we note that

$$\widehat{Vw}(p) \geq 8\pi a - Ca^3 p^2.$$

We find that $p^2 + 2(\rho_0 + t_0)\widehat{Vw}(p) \geq Cp^2$ for all $p$. Together with $\delta \geq 0$, this implies

$$\begin{aligned}(p^2+\delta)^2 &+ 2(p^2+\delta)(\rho_0+t_0)\widehat{Vw}(p) \\ &= (p^2+\delta)\left(p^2+\delta+2(\rho_0+t_0)\widehat{Vw}(p)\right) \geq Cp^4.\end{aligned}$$

In particular, this means there are no problems with the square root.

Using (5.17) in (5.16) we find for the minimizers

$$\begin{aligned}\gamma(p) &= \frac{\beta}{TG}(p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p)) - \frac{1}{2} \\ &= (e^{G(p)}-1)^{-1}\frac{p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p)}{\sqrt{(p^2+\delta)^2+2(p^2+\delta)(\rho_0+t_0)\widehat{Vw}(p)}} \\ &\qquad + \frac{1}{2}\left(\frac{p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p)}{\sqrt{(p^2+\delta)^2+2(p^2+\delta)(\rho_0+t_0)\widehat{Vw}(p)}} - 1\right) \\ \alpha(p) &= -\frac{\beta}{TG}(\rho_0+t_0)\widehat{Vw}(p) \\ &= -\left((e^{G(p)}-1)^{-1}+\frac{1}{2}\right)\frac{(\rho_0+t_0)\widehat{Vw}(p)}{\sqrt{(p^2+\delta)^2+2(p^2+\delta)(\rho_0+t_0)\widehat{Vw}(p)}}.\end{aligned}$$

These indeed satisfy $\alpha^2 \leq \gamma(\gamma+1)$. Inserting them into the functional we obtain

$$\begin{aligned}&(p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p))\gamma(p) + (\rho_0+t_0)\widehat{Vw}(p)\alpha(p) - Ts(\beta(p)) \\ &= \frac{\beta(p)}{TG(p)}(TG(p))^2 - \frac{1}{2}(p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p)) \\ &\qquad + T\beta(p)\ln\left(\frac{\beta(p)-\frac{1}{2}}{\beta(p)+\frac{1}{2}}\right) - \frac{1}{2}T\ln\left(\beta(p)^2-\frac{1}{4}\right) \\ &= -\frac{1}{2}(p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p)) + \frac{1}{2}TG(p) + T\ln(1-e^{-G(p)}) \\ &= T\ln(1-e^{-G(p)}) \\ &+ \frac{1}{2}\left(\sqrt{(p^2+\delta)^2+2(p^2+\delta)(\rho_0+t_0)\widehat{Vw}(p)} - (p^2+\delta+(\rho_0+t_0)\widehat{Vw}(p))\right),\end{aligned}$$

which gives the right expression. □

We summarize and rewrite the relevant quantities in the following corollary. The expressions may seem a bit involved, but it will turn out to be useful to write them in this way.

**Corollary 16.** *Let $-1 \leq \theta \leq 0$, $d \geq 0$, $\sigma \geq 0$, $\phi > 0$ and $0 \leq \rho_0 \leq \rho$ be fixed. Assume $\rho_0 a/\phi^2 = \sigma/8\pi$ and let $\delta = d\phi^2$, and $t_0 = \theta\rho_0$. We then have*

$$\begin{aligned}
&\mathcal{F}^{\mathrm{s}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) \\
&\quad = (2\pi)^{-3}\phi^5 \frac{1}{2}\int \Big[\sqrt{(p^2+d)^2 + 2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}} \\
&\qquad\qquad - (p^2 + d + (1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}) + \frac{((1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a})^2}{2p^2}\Big] dp \\
&\qquad + (2\pi)^{-3}T\phi^3 \int \ln\left(1 - e^{-\frac{\phi^2}{T}\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}}\right) dp - d\phi^2\rho_{\gamma^{\rho_0,\delta}} \\
&\quad =: F^{(1)} + F^{(2)} - d\phi^2\rho_{\gamma^{\rho_0,\delta}},
\end{aligned}$$

*where*

$$\begin{aligned}
\rho_{\gamma^{\rho_0,\delta}} &= (2\pi)^{-3}\phi^3\frac{1}{2}\int\left(\frac{p^2+d+(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}{\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}} - 1\right)dp \\
&\quad + (2\pi)^{-3}\phi^3\int\left(e^{\frac{\phi^2}{T}\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}} - 1\right)^{-1} \\
&\qquad\qquad \times \frac{p^2+d+(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}{\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}}dp \\
&=: \rho_\gamma^{(1)} + \rho_\gamma^{(2)}.
\end{aligned} \tag{5.18}$$

In the above, $\phi$ may seem superfluous, but we will use it later to allow for different scalings: we either choose $\phi = Ta$ or $\phi = \sqrt{\rho_0 a}$. This allows us to choose the parameters $\sigma, d$ and $\theta$ to be of order 1 in the different regimes.

5.3. **A priori estimates on the free Bose gas.** To establish that the error terms in Lemma 13 are small for the minimizer of the full functional, we need a priori estimates, which we will prove in the next subsection. To prepare for this, we prove some facts about the free Bose gas first.

Let $\gamma_{\mu(\rho)}$ denote the minimizer with density $\rho$ for the free gas functional

$$\mathcal{F}_0(\gamma) = (2\pi)^{-3}\int p^2\gamma(p) - Ts(\gamma(p), 0)dp.$$

More precisely, $\mu(\rho) \leq 0$ represents the chemical potential such that $\gamma_{\mu(\rho)}$ actually minimizes $\mathcal{F}_0(\gamma) - \mu(\rho)(2\pi)^{-3}\int\gamma$. If $\rho > \rho_{\mathrm{fc}}$ there is no minimizer with $(2\pi)^{-3}\int\gamma = \rho$ and $\mu(\rho) = 0$, i.e. we have the global free minimizer $\gamma_0$ with $(2\pi)^{-3}\int\gamma_0 = \rho_{\mathrm{fc}}$. We denote the minimizing energy $F_0(T,\rho) = \mathcal{F}_0(\gamma_{\mu(\rho)})$. The minimizer $\gamma_\mu$ is given by

$$\gamma_\mu(p) = \frac{1}{e^{(p^2-\mu)/T} - 1}, \tag{5.19}$$

hence

$$\rho = (2\pi)^{-3}T^{3/2}\int\left[e^{(p^2 - T^{-1}\mu(\rho))} - 1\right]^{-1}dp,$$

and the energy is

$$\begin{aligned} F_0(T,\rho) &= (2\pi)^{-3}T\int \ln\left(1-e^{-(p^2-\mu(\rho))/T}\right)dp + \mu(\rho)\rho \\ &= (2\pi)^{-3}T^{5/2}\int \ln\left(1-e^{-(p^2-T^{-1}\mu(\rho))}\right)dp + \mu(\rho)\rho. \end{aligned} \tag{5.20}$$

We see that we have the following scalings for $F_0$ and $\mu$:

$$F_0(T,\rho) = T^{5/2}f_0\left(\rho/T^{3/2}\right), \qquad \mu(\rho) = Tm\left(\rho/T^{3/2}\right),$$

where $f_0$ and $m$ are the functions independent of $T$ given by

$$f_0(n) = (2\pi)^{-3}\int \ln\left(1-e^{-(p^2-m(n))}\right)dp + m(n)n,$$

$$n = (2\pi)^{-3}\int \left[e^{p^2-m(n)}-1\right]^{-1}dp.$$

The critical density is $\rho_{\rm fc} = T^{3/2}n_{\rm fc}$, where

$$n_{\rm fc} = (2\pi)^{-3}\int \left[e^{p^2}-1\right]^{-1}dp = \left(8\pi^{3/2}\right)^{-1}\zeta(3/2). \tag{5.21}$$

The minimal free energy is $\min_\rho F_0(T,\rho) = T^{5/2}f_{\min}$, where

$$\begin{aligned} f_{\min} &= (2\pi)^{-3}\int \ln\left(1-e^{-p^2}\right)dp \\ &= -\frac{2}{3}(2\pi)^{-3}\int p^2\left[e^{p^2}-1\right]^{-1}dp = -\left(8\pi^{3/2}\right)^{-1}\zeta(5/2). \end{aligned}$$

The second identity can for example be seen by putting back in the $T$ dependence, differentiating $\int \ln(1-e^{-p^2/T})dp$ with respect to $T$ directly under the integral sign, and also noticing that it is $\frac{3}{2}T^{-1}$ times the integral.

We now prove two estimates that we will use in the next section.

**Lemma 17.** *There exist constants $c_1, C_1 > 0$ such that for all $n$ we have*

$$f_0(n) \leq f_{\min} + C_1[n_{\rm fc}-n]_+^3, \tag{5.22}$$

*and for all $n_1 \leq n_2 \leq n_{\rm fc}$*

$$f_0(n_1) \geq f_0(n_2) + c_1(n_2-n_1)^3. \tag{5.23}$$

*Also, given $n_0 < n_{\rm fc}$, there exists $c_0 > 0$ such that for all $n_0 \leq n \leq n_{\rm fc}$*

$$f_0(n) \leq f_0(n_0) - c_0(n-n_0)(n_{\rm fc}-n_0)^2. \tag{5.24}$$

*Proof.* Let us analyse how the energy $f_0(n)$ goes up if $n = n_{\rm fc} - \delta n$ for $\delta n > 0$. For simplicity we set $\lambda = -m(n) \geq 0$. We then have

$$\begin{aligned} \delta n &= (2\pi)^{-3}\left(\int [e^{p^2}-1]^{-1} - [e^{p^2+\lambda}-1]^{-1}dp\right) \\ &= (2\pi)^{-3}\lambda^{3/2}\left(\int [e^{\lambda p^2}-1]^{-1} - [e^{\lambda(p^2+1)}-1]^{-1}dp\right) \\ &= (2\pi)^{-3}\lambda^{1/2}\left(\int (|p|^{-2}-(|p|^2+1)^{-1})dp + o(1)\right) = (4\pi)^{-1}\lambda^{1/2} + o(\lambda^{1/2}) \end{aligned} \tag{5.25}$$

as $\lambda \to 0$. We then find for the energy

$$\begin{aligned}
&(2\pi)^{-3}\int \ln(1-e^{-(p^2+\lambda)})dp - \lambda(2\pi)^{-3}\int [e^{p^2+\lambda}-1]^{-1}dp \\
&= (2\pi)^{-3}\int \ln(1-e^{-p^2})dp \\
&\quad +(2\pi)^{-3}\lambda^{3/2}\int \ln(1-e^{-\lambda(p^2+1)}) - \ln(1-e^{-\lambda p^2}) - \lambda[e^{\lambda(p^2+1)}-1]^{-1}dp \\
&= f_{\min} + (2\pi)^{-3}\lambda^{3/2}\left(\int \ln(1+|p|^{-2}) - (p^2+1)^{-1}dp + o(1)\right) \\
&= f_{\min} + (12\pi)^{-1}\lambda^{3/2} + o(\lambda^{3/2})
\end{aligned}$$

as $\lambda \to 0$. We thus conclude that

$$f_0(n) = f_{\min} + \frac{16\pi^2}{3}[n_{\rm fc}-n]_+^3 + o([n_{\rm fc}-n]_+^3) \tag{5.26}$$

as $[n_{\rm fc}-n]_+ \to 0$. This proves the statement. We also see that the free Bose gas has a third-order phase transition between the condensed and non-condensed phase.

The final statement is found by combining (5.26) with the fact that $f_0(n)$ is convex and strictly decreasing in $0 \le n \le n_{\rm fc}$. □

5.4. **A priori estimates.** In this section, we always assume that $T \le D\rho^{2/3}$ for some fixed constant $D$. The estimates below will depend on $D$.

Our goal will be to acquire some tools to approximate the free energy functional (2.1) in the dilute limit $\rho^{1/3}a \ll 1$. Propositions 19, 21 and 23 provide a priori bounds for the terms involving $\gamma$ and $\widehat{V}$. The first estimate holds in general for $T \le D\rho^{2/3}$. The two other estimates are sharper and provide bounds at densities very close to the free critical density where, according to Subsection 5.5, the phase transition has to occur. This means that we can zoom in on this region and analyse the nature of the minimizers there. This will be done in Subsection 5.7.

Let $(\gamma, \alpha, \rho_0 = \rho - \rho_\gamma)$ be a minimizing triple for (2.5) at a temperature $T$.

Using the bound $\widehat{V}(p) \le \widehat{V}(0)$ we find the following upper bound in terms of the free gas energy $\mathcal{F}_0$

$$\begin{aligned}
\mathcal{F}^{\rm can}(\gamma,\alpha,\rho_0) &\le \mathcal{F}^{\rm can}(\gamma_{\mu(\rho)}, 0, [\rho-\rho_{\rm fc}]_+) \\
&\le \mathcal{F}_0(\gamma_{\mu(\rho)}) + \rho^2\widehat{V}(0) - \frac{1}{2}[\rho-\rho_{\rm fc}]_+^2\widehat{V}(0).
\end{aligned} \tag{5.27}$$

We also have

$$\begin{aligned}
\mathcal{F}^{\rm can}(\gamma,\alpha,\rho_0) \ge{}& \mathcal{F}_0(\gamma) + \frac{1}{2}\widehat{V}(0)\rho^2 + \rho_0(2\pi)^{-3}\int \widehat{V}(p)\gamma(p)dp \\
&+ \frac{1}{2}(2\pi)^{-6}\iint \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \frac{1}{2}\rho_0^2\widehat{V}(0),
\end{aligned} \tag{5.28}$$

where we have first used that the entropy decreases if we replace $\alpha$ by 0 and then minimized over $\alpha$, finding the minimizer $\alpha = -(2\pi)^3\rho_0\delta_0$. As

$\rho_\gamma, \rho_0 \leq \rho$ and the free gas energy is non-increasing we conclude the following preliminary estimate

$$\mathcal{F}_0(\gamma_{\mu(\rho_\gamma)}) \leq \mathcal{F}_0(\gamma) \leq \mathcal{F}_0(\gamma_{\mu(\rho)}) + \rho^2 \widehat{V}(0). \tag{5.29}$$

We will use this to give an estimate on the integral of $\gamma$ in a region $|p| > b$, where $b$ is to be chosen below. We shall use the following result.

**Lemma 18** (A priori kinetic energy bound). *If for some $Y > 0$ the function $\gamma$ satisfies $\mathcal{F}_0(\gamma) \leq \mathcal{F}_0(\gamma_{\mu(\rho_\gamma)}) + Y$, then for all $b$ with $b^2 > 8T$ we have*

$$\frac{1}{2}(2\pi)^{-3} \int_{|p|>b} p^2 \gamma(p) dp \leq Y + CT^{5/2} e^{-b^2/4T}.$$

*Proof.* Using the fact that $\mu(\rho_\gamma) \leq 0$ and $\mu(\rho_\gamma)(2\pi)^{-3} \int \gamma_{\mu(\rho_\gamma)} = \mu(\rho_\gamma)\rho_\gamma$, the result follows from

$$\begin{aligned}
\mathcal{F}_0(\gamma) - \mu(\rho_\gamma)\rho_\gamma \geq\ & (2\pi)^{-3} \int_{|p|<b} \left(p^2\gamma(p) - Ts(\gamma(p), 0) - \mu(\rho_\gamma)\gamma(p)\right) dp \\
& + \frac{1}{2}(2\pi)^{-3} \int\limits_{|p|>b} p^2\gamma(p) dp + \frac{1}{2}(2\pi)^{-3} \int\limits_{|p|>b} \left(p^2\gamma(p) - 2Ts(\gamma(p), 0)\right) dp \\
\geq\ & (2\pi)^{-3} \int \left(p^2 \gamma_{\mu(\rho_\gamma)}(p) - Ts(\gamma_{\mu(\rho_\gamma)}(p), 0) - \mu(\rho_\gamma)\gamma_{\mu(\rho_\gamma)}(p)\right) dp \\
& + \frac{1}{2}(2\pi)^{-3} \int_{|p|>b} p^2\gamma(p) dp + (2\pi)^{-3} T \int_{|p|>b} \ln(1 - e^{-p^2/2T}) dp \\
\geq\ & \mathcal{F}_0(\gamma_{\mu(\rho_\gamma)}) - \mu(\rho_\gamma)\rho_\gamma + \frac{1}{2}(2\pi)^{-3} \int_{|p|>b} p^2\gamma(p) - CT^{5/2} e^{-b^2/4T},
\end{aligned}$$

which holds for $b^2 > 8T$, since then

$$\begin{aligned}
\int_{|p|>b} \ln(1 - e^{-p^2/2T}) dp \geq -C \int_{|p|>b} e^{-p^2/2T} dp \geq -Ce^{-b^2/4T} \int e^{-p^2/4T} dp \\
= -CT^{3/2} e^{-b^2/4T}.
\end{aligned}$$

□

Since $\mathcal{F}_0(\gamma_{\mu(\rho_\gamma)}) \geq \mathcal{F}_0(\gamma_{\mu(\rho)})$, we can use this lemma with $Y = \rho^2 \widehat{V}(0)$ to conclude from (5.29) that

$$\begin{aligned}
\iint_{|p-q|>2b} \gamma(p)\widehat{V}(p-q)\gamma(q) dp dq \leq C\widehat{V}(0)\rho \int_{|p|>b} \gamma(p) dp \\
\leq C\widehat{V}(0)\rho(\rho^2 \widehat{V}(0) + T^{5/2} e^{-b^2/4T}) b^{-2}.
\end{aligned} \tag{5.30}$$

We choose $b = a^{-1}(\rho^{1/3}a)^{3/4}$. Then $b^2/T \geq D^{-1}(\rho^{1/3}a)^{-1/2} \gg 1$ and we find

$$\iint_{|p-q|>2b} \gamma(p)\widehat{V}(p-q)\gamma(q) dp dq \leq C\rho^3 \widehat{V}(0)^2 b^{-2} \leq C\rho^2 a(\rho^{1/3}a)^{3/2}. \tag{5.31}$$

Of course, the same bound holds if $\widehat{V}(p-q)$ is replaced by $\widehat{V}(0)$. On the other hand we also have

$$\iint_{|p-q|<2b} \gamma(p)|\widehat{V}(p-q) - \widehat{V}(0)|\gamma(q) dp dq \leq Cb^2 \|\partial^2 \widehat{V}\|_\infty \rho^2 \leq C\rho^2 a(\rho^{1/3}a)^{3/2}. \tag{5.32}$$

For the same choice of $b$:

$$\left|\int \gamma(p)\widehat{V}(p)dp - \widehat{V}(0)\int \gamma(p)dp\right| \leq \left|\left(\int_{|p|\leq b} + \int_{|p|>b}\right)\gamma(p)\left(\widehat{V}(p)-\widehat{V}(0)\right)dp\right|$$
$$\leq Cb^2\|\partial^2\widehat{V}\|_\infty \int_{|p|\leq b}\gamma(p)dp + C\widehat{V}(0)b^{-2}\int_{|p|>b}p^2\gamma(p)dp$$
$$\leq C\rho a^3 b^2 + Cab^{-2}(\rho^2 a + T^{5/2}e^{-b^2/4T}) \leq C\rho a(\rho^{1/3}a)^{3/2}, \tag{5.33}$$

The same bounds hold for $\widehat{Vw}$ by (5.8). We have thus shown the following result.

**Proposition 19** (A priori estimates on $E_2$ and $E_4$)**.** *Any minimizing triple $(\gamma, \alpha, \rho_0)$ with density $\rho = \rho_\gamma + \rho_0$ and temperature $T$ satisfying $T < D\rho^{2/3}$ obeys the estimates*

$$\left|(2\pi)^{-6}\iint \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \widehat{V}(0)\rho_\gamma^2\right| \leq C\rho^2 a(\rho^{1/3}a)^{3/2},$$
$$\left|(2\pi)^{-3}\int \gamma(p)\widehat{V}(p)dp - \widehat{V}(0)\rho_\gamma\right| \leq C\rho a(\rho^{1/3}a)^{3/2},$$

*where the constant $C$ depends on $D$ and the potential $V$. This also holds with $\widehat{V}$ replaced by $\widehat{Vw}$.*

From (5.27), (5.28), and Proposition 19 we find that

$$\mathcal{F}_0(\gamma_{\mu(\rho)}) \geq \mathcal{F}_0(\gamma) + \frac{1}{2}[\rho - \rho_{\text{fc}}]_+^2\widehat{V}(0) - \rho_0^2\widehat{V}(0) - C\rho^2 a(\rho^{1/3}a)^{3/2}, \tag{5.34}$$

which implies

$$\rho_0^2\widehat{V}(0) \geq \frac{1}{2}[\rho - \rho_{\text{fc}}]_+^2\widehat{V}(0) - C\rho^2 a(\rho^{1/3}a)^{3/2}. \tag{5.35}$$

We thus get the following result.

**Lemma 20.** *If $(\gamma, \alpha, \rho_0)$ is a minimizing triple with $\rho = \rho_\gamma + \rho_0$ satisfying*

$$\rho > \rho_{\text{fc}} + C\rho(\rho^{1/3}a)^{3/4},$$

*then $\rho_0 \neq 0$.*

It follows that phase transition can only take place for

$$\rho \leq \rho_{\text{fc}} + C\rho(\rho^{1/3}a)^{3/4} \leq \rho_{\text{fc}} + C'\rho_{\text{fc}}(\rho_{\text{fc}}^{1/3}a)^{3/4}.$$

Hence from now on we consider only

$$\rho \leq \rho_{\text{fc}} + C'\rho_{\text{fc}}(\rho_{\text{fc}}^{1/3}a)^{3/4}. \tag{5.36}$$

Under this condition we shall give an upper bound on $\rho_0$.

If $\rho_0 > 2C'\rho_{\text{fc}}(\rho_{\text{fc}}^{1/3}a)^{3/4}$, then $\rho_\gamma = \rho - \rho_0 \leq \rho_{\text{fc}} - \frac{1}{2}\rho_0$ and thus

$$\begin{aligned}\mathcal{F}_0(\gamma_{\mu(\rho)}) &\geq \mathcal{F}_0(\gamma) - \widehat{V}(0)\rho_0^2 - C\rho_{\text{fc}}^2 a(\rho_{\text{fc}}^{1/3}a)^{3/2} \\ &\geq \mathcal{F}_0(\gamma_{\mu(\rho)}) + cT^{-2}\rho_0^3 - \widehat{V}(0)\rho_0^2 - C\rho_{\text{fc}}^2 a(\rho_{\text{fc}}^{1/3}a)^{3/2},\end{aligned} \tag{5.37}$$

where we have used the lower bound in (5.23) with $n_1 = T^{-3/2}\rho_\gamma$ and $n_2 = T^{-3/2}\min\{\rho, \rho_{\text{fc}}\}$. We conclude that $\rho_0 < C\rho_{\text{fc}}(\rho_{\text{fc}}^{1/3}a)^{5/6}$, which, in the dilute limit, contradicts the assumption $\rho_0 > 2C'\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{3/4}$. We conclude that (5.36) implies

$$\rho_0 \le 2C'\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{3/4}.$$

If we insert this bound into (5.34), we obtain

$$\mathcal{F}_0(\gamma_{\mu(\rho)}) \ge \mathcal{F}_0(\gamma) - C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2}. \tag{5.38}$$

Since $\mathcal{F}_0(\gamma_{\mu(\rho)}) \le \mathcal{F}_0(\gamma_{\mu(\rho_\gamma)})$, we use Lemma 18 with $Y = Ca\rho_{\rm fc}^2(\rho_{\rm fc}^{1/3}a)^{3/2}$, and, as in (5.30), arrive at

$$\iint_{|p-q|>2b} \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq \le C\widehat{V}(0)\rho(a\rho_{\rm fc}^2(\rho_{\rm fc}^{1/3}a)^{3/2} + T^{5/2}e^{-b^2/4T})b^{-2}. \tag{5.39}$$

We choose $b = a^{-1}(\rho_{\rm fc}^{1/3}a)^{3/4}$, such that $b^2/T \ge c(\rho_{\rm fc}^{1/3}a)^{-1/2} \gg 1$. The error above is then $C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^3$. This time we can expand $\widehat{V}$ to second order

$$\iint_{|p-q|<2b} \gamma(p)|\widehat{V}(p-q) - \widehat{V}(0) - \frac{1}{6}\Delta\widehat{V}(0)(p-q)^2|\gamma(q)dpdq \le Cb^3 \sup|\partial^3\widehat{V}|\rho^2$$
$$= Cb^3a^4\rho^2 \le C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{2+1/4}.$$

Note that the integrals of the terms involving $\widehat{V}(0)$ and $\Delta\widehat{V}(0)$ over $\{|p-q| > 2b\}$ can be estimated with Lemma 18 like (5.39), that all these bounds can also be derived for $\int \widehat{V}(p)\gamma(p)dp$, and that we can derive similar bounds for $\widehat{Vw}$ using (5.8), so that we arrive at the following improvement of Proposition 19.

**Proposition 21.** *Any minimizing triple $(\gamma, \alpha, \rho_0)$ with density $\rho = \rho_\gamma + \rho_0$ and temperature $T$ satisfying $D^{-3/2}T^{3/2} < \rho < \rho_{\rm fc} + C'\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{3/4}$ obeys the estimates*

$$\left|(2\pi)^{-6}\iint \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \widehat{V}(0)\rho_\gamma^2 - \frac{1}{3(2\pi)^3}\Delta\widehat{V}(0)\rho_\gamma\int p^2\gamma(p)dp\right| \le C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{2+1/4} \tag{5.40}$$

*and*

$$\left|(2\pi)^{-3}\int \widehat{V}(p)\gamma(p)dp - \widehat{V}(0)\rho_\gamma - \frac{1}{6(2\pi)^3}\Delta\widehat{V}(0)\int p^2\gamma(p)dp\right| \le C\rho_{\rm fc}a(\rho_{\rm fc}^{1/3}a)^{2+1/4},$$

*where the constants $C$ depend on $D$ and the potential $V$ This also holds with $\widehat{V}$ replaced by $\widehat{Vw}$.*

We are now ready to prove two more results. First, we provide an upper bound on $\rho_0$ and one on densities where a phase transition can occur ('critical densities'), which will be matched with a lower bound in the next section to show that there is no phase transition outside the region $|\rho - \rho_{\rm fc}| < C\rho(\rho^{1/3}a)$. The second is an a priori estimate on the error $E_5$.

**Lemma 22** (Upper bound on critical densities and $\rho_0$)**.** *Assume that the density $\rho = \rho_0 + \rho_\gamma$ and temperature $T$ satisfy $D^{-3/2}T^{3/2} < \rho < \rho_{\rm fc} + C'\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{3/4}$. Then,*

- $\rho_0 < C\rho(\rho^{1/3}a)$.
- *there exists a constant $C$ such that any minimizing triple with $\rho > \rho_{\rm fc} + C\rho(\rho^{1/3}a)$ has $\rho_0 \neq 0$.*

*Proof.* For $|\delta| < 1$ (both positive and negative) we find using the scaling of the free gas energy that

$$\mathcal{F}_0(\gamma) \geq (2\pi)^{-3}\delta \int p^2\gamma(p)dp + (1-\delta)^{-3/2}\mathcal{F}_0(\gamma_0). \tag{5.41}$$

Since $\mathcal{F}_0(\gamma) \leq C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2}$ by (5.38) and $\mathcal{F}(\gamma_0) \leq 0$, it follows that

$$\int p^2\gamma(p)dp \leq C\rho^{5/3}. \tag{5.42}$$

Together with Proposition 21, this implies that

$$(2\pi)^{-6}\iint \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq = \widehat{V}(0)\rho_\gamma^2 + O(\rho^2 a(\rho^{1/3}a)^2)$$

and

$$(2\pi)^{-3}\int \widehat{V}(p)\gamma(p)dp = \widehat{V}(0)\rho_\gamma + O(\rho a(\rho^{1/3}a)^2).$$

These two bounds together with (5.27) and (5.28) yield

$$\begin{aligned}\mathcal{F}_0(\gamma_{\mu(\rho)}) + \rho^2\frac{\widehat{V}(0)}{2} - \frac{1}{2}[\rho-\rho_{\rm fc}]_+^2\widehat{V}(0) \geq \\ \mathcal{F}_0(\gamma) + \rho_0\rho_\gamma\widehat{V}(0) + \frac{\widehat{V}(0)}{2}\rho_\gamma^2 - \frac{\widehat{V}(0)}{2}\rho_0^2 + O(\rho^2(\rho^{1/3}a)^2),\end{aligned} \tag{5.43}$$

and so

$$\rho_0^2 \geq \frac{1}{2}[\rho-\rho_{\rm fc}]_+^2 - C\rho^2(\rho^{1/3}a)^2,$$

which implies the second statement. We also notice that (5.43) and (5.23) (used as in (5.37)) imply

$$CT^{-2}\rho_0^3 - \widehat{V}(0)\rho_0^2 - Ca\rho^2(\rho^{1/3}a)^2 \leq 0,$$

which proves the first statement. □

**Proposition 23** (A priori estimate on $E_5$)**.** *Let $(\gamma, \alpha, \rho_0)$ be a minimizing triple with density $\rho = \rho_\gamma + \rho_0$ such that $|\rho - \rho_{\rm fc}| < C\rho(\rho^{1/3}a)$. Also assume $T < D\rho^{2/3}$. Then*

$$(2\pi)^{-6}\iint \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq = \widehat{V}(0)\rho_\gamma^2 + \frac{\zeta(3/2)\zeta(5/2)}{128\pi^3}\Delta\widehat{V}(0)T^4 + o(T^4a^3).$$

*Proof.* First notice that

$$\frac{\zeta(3/2)\zeta(5/2)}{128\pi^3}\Delta\widehat{V}(0)T^4 = \frac{\Delta\widehat{V}(0)}{3(2\pi)^6}\int p^2(e^{p^2/T}-1)^{-1}dp\int(e^{p^2/T}-1)^{-1}dp, \tag{5.44}$$

so that according to (5.40) it is enough to show that

$$\frac{1}{3}\Delta\widehat{V}(0)\rho_\gamma\int p^2\gamma(p)dp = \frac{1}{3(2\pi)^3}\Delta\widehat{V}(0)\int\gamma_0(p)dp\int p^2\gamma_0(p)dp + o(T^4a^3). \tag{5.45}$$

We have

$$\left|\rho_\gamma\int p^2\gamma(p)dp - \rho_{\rm fc}\int p^2\gamma_0(p)dp\right| \leq$$
$$|\rho_\gamma - \rho_{\rm fc}|\int p^2\gamma(p)dp + \rho_{\rm fc}\left|\int p^2(\gamma(p)-\gamma_0(p))dp\right|.$$

The first statement in Lemma 22, combined with the assumptions, implies

$$|\rho_\gamma - \rho_{\rm fc}| \leq \rho_0 + |\rho - \rho_{\rm fc}| \leq C\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a).$$

This and (5.42) allow us to bound the first contribution to the difference in (5.45):

$$\Delta\widehat{V}(0)|\rho_\gamma - \rho_{\rm fc}|\int p^2\gamma(p)dp \leq C\rho_{\rm fc}^3a^4 = o(T^4a^3).$$

To bound the other contribution, we use (5.41). We do the same for $\gamma_0$, but with $-\delta$. Putting these two bounds together yields

$$(2\pi)^{-3}\delta\int p^2(\gamma(p)-\gamma_0(p))dp \leq \mathcal{F}_0(\gamma)+\mathcal{F}_0(\gamma_0)-((1-\delta)^{-3/2}+(1+\delta)^{-3/2})\mathcal{F}_0(\gamma_0).$$

Writing (5.22) and (5.38) in succession gives

$$\mathcal{F}_0(\gamma_0) + CT^{-2}[\rho_{\rm fc}-\rho]_+^3 \geq \mathcal{F}_0(\gamma_{\mu(\rho)}) \geq \mathcal{F}_0(\gamma) - C\rho_{\rm fc}^2a(\rho_{\rm fc}^{1/3}a)^{3/2},$$

which implies

$$CT^{5/2}\rho_{\rm fc}a^3 + C\rho_{\rm fc}^2a(\rho_{\rm fc}^{1/3}a)^{3/2} \geq 0.$$

Thus

$$\begin{aligned}\frac{\delta}{(2\pi)^3}\int p^2(\gamma(p)-\gamma_0(p))dp &\leq -((1-\delta)^{-\frac{3}{2}} + (1+\delta)^{-\frac{3}{2}} - 2)\mathcal{F}_0(\gamma_0)\\ &\quad + CT^{5/2}\rho_{\rm fc}a^3 + C\rho_{\rm fc}^2a(\rho_{\rm fc}^{1/3}a)^{3/2}\\ &\leq C\delta^2T^{5/2} + CT^{5/2}\rho_{\rm fc}a^3 + CT^{5/2}(\rho_{\rm fc}^{1/3}a)^{5/2}.\end{aligned}$$

By choosing $|\delta| = (\rho_{\rm fc}^{1/3}a)^{5/4}$, we finally obtain

$$\int p^2(\gamma(p)-\gamma_0(p))dp \leq CT^{5/2}(\rho_{\rm fc}^{1/3}a)^{5/4},$$

which implies

$$\Delta\widehat{V}(0)\rho_{\rm fc}\left|\int p^2(\gamma(p)-\gamma_0(p))dp\right| \leq Ca^3T^4(\rho_{\rm fc}^{1/3}a)^{5/4} = o(T^4a^3).$$

This completes the proof. □

5.5. **Estimate on critical densities.** In this section, we provide a lower bound on densities where a phase transition can occur. Together with the upper bound from Lemmas 20 and 22, we obtain the following a priori estimate.

**Proposition 24** (Estimate on critical densities)**.** *There exists a constant $C_0$ such that for any minimizing triple:*

(1) $\rho_0 \neq 0$ *if* $\rho > \rho_{\mathrm{fc}} + C_0\rho_{\mathrm{fc}}(\rho_{\mathrm{fc}}^{1/3}a)$*;*
(2) $\rho_0 = 0$ *if* $\rho < \rho_{\mathrm{fc}} - C_0\rho_{\mathrm{fc}}(\rho_{\mathrm{fc}}^{1/3}a)$*.*

*Proof of the second statement. (The first follows from Lemmas 20 and 22.)* *Step 1.* We will first consider temperatures $T \leq D\rho^{2/3}$, so that we can use the a priori estimates proved in the previous section, and comment on higher temperatures in the final step.

We are interested in the canonical minimization problem (2.5), but our strategy will be to use the grand canonical formulation of the problem. This is not straightforward since the canonical energy is not necessarily convex in $\rho$ (it will indeed turn out not to be as we prove in Subsection 5.7).

As a first step, we simply assume the correspondence between canonical and grand canonical is obvious. That is, given $\rho$, there is a $\mu$ such that the canonical minimizing triple $(\gamma, \alpha, \rho_0)$ with $\rho_0 + \rho_\gamma = \rho$ is a minimizer of the grand canonical functional (2.1) with that $\mu$ (which will not be the case in general.) In [25], it was shown that $\gamma$ satisfies the Euler–Lagrange equation

$$p^2 - \mu + \rho\widehat{V}(0) + \rho_0\widehat{V}(p) + (2\pi)^{-3}\widehat{V} * \gamma(p) - T\frac{\gamma + \frac{1}{2}}{\beta}\ln\frac{\beta + \frac{1}{2}}{\beta - \frac{1}{2}} = 0.$$

Since $\beta = \sqrt{(\gamma + \frac{1}{2})^2 - \alpha^2}$, it follows that

$$p^2 - \mu + \rho\widehat{V}(0) + \rho_0\widehat{V}(p) + (2\pi)^{-3}\widehat{V} * \gamma(p) - T\ln\frac{\gamma + 1}{\gamma} \geq 0,$$

which implies

$$\gamma(p) \geq \left[\exp\left(\frac{p^2 - \mu + \rho\widehat{V}(0) + \rho_0\widehat{V}(p) + (2\pi)^{-3}\widehat{V} * \gamma(p)}{T}\right) - 1\right]^{-1}. \tag{5.46}$$

The same argument as in (5.28) implies that

$$\mathcal{F}(\gamma, \alpha, \rho_0) \geq \mathcal{F}(\gamma, 0, 0) + \rho_0\left((2\pi)^{-3}\int \widehat{V}(p)\gamma(p)dp + \rho_\gamma\widehat{V}(0) - \mu\right).$$

Thus, if the minimizer has $\rho_0 > 0$, then we need to have

$$(2\pi)^{-3}\int \widehat{V}(p)\gamma(p)dp + \rho_\gamma\widehat{V}(0) - \mu \leq 0.$$

Using this in (5.46), we obtain

$$\gamma(p) \geq \left[\exp\left(\frac{p^2 + Ca\rho(\rho^{1/3}a)}{T}\right) - 1\right]^{-1}, \tag{5.47}$$

where we also used the first statement in Lemma 22 and Proposition 19. Given the claim we are trying to prove, we can assume $\rho \leq \rho_{\text{fc}}$, so that, using a change of variables and the fact that $\rho_0 > 0$, we have

$$\rho_\gamma \geq T^{3/2} \int \left[\exp\left(p^2 + C(\rho^{1/3}a)^2\right) - 1\right]^{-1} dp \geq \rho_{\text{fc}}(1 - C(\rho^{1/3}a)),$$

where we used (5.25). We conclude that there exists a constant $C_1$ such that $\rho_0 = 0$ for any minimizing triple with $\rho < \rho_{\text{fc}} - C_1\rho_{\text{fc}}(\rho_{\text{fc}}^{1/3}a)$ satisfying the extra assumption that there is a $\mu$ that will give the same minimizer of the grand canonical problem. This will, however, not be the case in general because the canonical energy may not be convex in $\rho$.

*Step 2.* Given a $\rho$, there are $\rho_\pm$ such that $\rho_- \leq \rho \leq \rho_+$ and such that the convex hull of $F^{\text{can}}$ is linear on the interval $[\rho_-, \rho_+]$. To see this, we first use that $\rho_0 = 0$ for small $\rho$, as established in [25]. Together with the fact that the canonical functional with $\rho_0 = 0$ is strictly convex, this implies that the canonical energy is convex for small $\rho$. The simple lower bound

$$F^{\text{can}}(T, \rho) \geq -CT^{5/2} - \frac{1}{2}\rho_0 \int \widehat{V} + \frac{1}{2}\widehat{V}(0)\rho^2$$

then confirms the existence of $\rho_-$ and $\rho_+$.

The assumption made in the previous step will hold for $\rho_\pm$, i.e. $\rho_+$ and $\rho_-$ correspond to a minimum for the grand canonical functional for some (shared) $\mu$ that is the slope of $F^{\text{can}}$ on $[\rho_-, \rho_+]$, and the conclusion from step 1 above holds for these densities. Since $\rho_- \leq \rho$, this implies that if we choose $C_0 \geq C_1$ then $\rho_{0-} = 0$ for the total density $\rho_-$.

If the density $\rho_+$ also satisfies a corresponding upper bound, then $\rho_{0+} = 0$ as well. In that case, as the canonical functional with $\rho_0 = 0$ is strictly convex, we conclude that in the interval $[\rho_-, \rho_+]$ we must have $\rho_0 = 0$ and hence $\rho_- = \rho_+ = \rho$.

Let $\mu$ be the slope of the convex hull of $F^{\text{can}}$ on $[\rho_-, \rho_+]$ (where it is linear). By the $\rho_0$-Euler–Lagrange equation for the grand canonical functional (2.1), it follows that

$$\mu \leq \rho_-\widehat{V}(0) + (2\pi)^{-3} \int \widehat{V}\gamma_- \leq 2\rho_-\widehat{V}(0) \leq 2\rho_{\text{fc}}(1 - C_0\rho_{\text{fc}}^{1/3}a)\widehat{V}(0).$$

The aim is to prove that $\rho_+ < \rho_{\text{fc}} - C_1\rho_{\text{fc}}(\rho_{\text{fc}}^{1/3}a)$ by proving an upper bound on any density minimizing the grand canonical functional with $\mu$ satisfying the bound above. As the minimizing density increases with $\mu$, we can assume that

$$\mu = 2\rho_{\text{fc}}(1 - C_0\rho_{\text{fc}}^{1/3}a)\widehat{V}(0). \tag{5.48}$$

Recall that $C_0$ is a constant that we will choose large enough to get the proof to work. Our choice for $C_0$ will be universal, so that we can make the a priori assumption that $C_0\rho_{\text{fc}}^{1/3}a \leq 1$.

*Step 3.* Let $\mu$ be as in (5.48). We will now first show the a-priori bound $\rho \leq C\rho_{\text{fc}}$. From (5.14), the definition of $\mathcal{F}^{\text{sim}}$ (5.1) and the definition of $\mathcal{F}^{\text{S}}$

(5.15), we find that

$$\begin{aligned}\mathcal{F}(\gamma,\alpha,\rho_0) &= \mathcal{F}^{\mathrm{S}}(\gamma,\alpha,\rho_0)-\mu\rho\\ &\quad+\frac{1}{2}\widehat{V}(0)\rho_\gamma^2+\widehat{V}(0)\rho_0\rho_\gamma-(\rho_0+t_0)(2\pi)^{-3}\int\widehat{Vw}(p)\gamma(p)dp\\ &\quad+(2\pi)^{-3}\rho_0\int\widehat{V}(p)\gamma(p)dp-4\pi a(\rho_0+t_0)^2+8\pi a(\rho_0+t_0)\rho_0\\ &\quad+\frac{1}{2}(2\pi)^{-6}\iint\gamma(p)\widehat{V}(p-q)\gamma(q)dpdq \qquad (5.49)\\ &\quad+\frac{1}{2}(2\pi)^{-6}\iint(\alpha(p)-\alpha_0(p))\widehat{V}(p-q)(\alpha(p)-\alpha_0(p))dpdq.\end{aligned}$$

We now choose $0\geq t_0\geq-\rho_0$. If $8\pi a\rho_0\leq 4\rho_{\mathrm{fc}}\widehat{V}(0)$ we choose $t_0=0$. Note that in this case we already have an upper bound $\rho_0\leq C\rho_{\mathrm{fc}}$, and the argument below will give the desired result for $\rho_\gamma$. Otherwise we choose

$$8\pi a(t_0+\rho_0)=4\rho_{\mathrm{fc}}\widehat{V}(0)>2\mu$$

by the assumption (5.48) on $\mu$. We now give a lower bound by ignoring the last two integrals, the second term in the second line, and the first term in the third line in (5.49). Finally we minimize $\mathcal{F}^{\mathrm{s}}$ using Lemma 22 with $\delta=0$.

We first consider the last integral in the expression for the minimum of $\mathcal{F}^{\mathrm{s}}$. We know from the assumptions made at the start of Sections 3 and 4 that

$$|\widehat{Vw}(p)|\leq\widehat{Vw}(0)=8\pi a,\quad \widehat{Vw}(p)\geq 8\pi a-Ca^3p^2, \qquad (5.50)$$

where the first inequality follows since $Vw$ is positive. The only negative contribution to the last integral therefore comes from the region $|p|>C/a$. For such $p$ we have that

$$(\rho_0+t_0)|\widehat{Vw}(p)|/p^2\leq C\rho_{\mathrm{fc}}a^3\ll 1.$$

Hence the last integral can be estimated below by

$$-C(\rho_0+t_0)^3\int_{|p|>1/a}\frac{|\widehat{Vw}(p)|^3}{p^4}\geq -C\rho_{\mathrm{fc}}^3a^4=-C\rho_{\mathrm{fc}}^2a(\rho_{\mathrm{fc}}a^3).$$

This argument will again be used in the next step to bound this integral.

The first integral with $G$ can be bounded below by replacing $G$ with a lower bound. We use again (5.50):

$$G=T^{-1}\sqrt{p^4+2(\rho_0+t_0)p^2\widehat{Vw}(p)}\geq T^{-1}p^2\sqrt{1-C\rho_{\mathrm{fc}}a^3}.$$

Altogether, we arrive at a lower bound

$$\begin{aligned}\mathcal{F}(\gamma,\alpha,\rho_0) &\geq \mathcal{F}_0(\gamma_0)(1+C\rho_{\mathrm{fc}}a^3)-\mu\rho_\gamma-\mu\rho_0\\ &\quad+\frac{1}{2}\widehat{V}(0)\rho_\gamma^2-Ca\rho_{\mathrm{fc}}\rho_\gamma-Ca\rho_{\mathrm{fc}}^2+4\rho_{\mathrm{fc}}\widehat{V}(0)\rho_0-C\rho_{\mathrm{fc}}^3a^4\\ &\geq \mathcal{F}_0(\gamma_0)-C\rho_{\mathrm{fc}}^{8/3}a^3-2\rho_{\mathrm{fc}}\widehat{V}(0)\rho_\gamma+\frac{1}{2}\widehat{V}(0)\rho_\gamma^2\\ &\quad-Ca\rho_{\mathrm{fc}}\rho_\gamma+2\rho_{\mathrm{fc}}\widehat{V}(0)\rho_0-Ca\rho_{\mathrm{fc}}^2-C\rho_{\mathrm{fc}}^3a^4,\end{aligned}$$

where $\gamma_0$ is the minimizer of the free gas functional. By inserting $\gamma_0$ and $\alpha = \rho_0 = 0$ into $\mathcal{F}$ we get the upper bound

$$\mathcal{F}_0(\gamma_0) - \mu\rho_{\rm fc} + \widehat{V}(0)\rho_{\rm fc}^2 \leq \mathcal{F}_0(\gamma_0) - \widehat{V}(0)\rho_{\rm fc}^2 + 2D\rho_{\rm fc}^2\widehat{V}(0)(\rho_{\rm fc}^{1/3}a).$$

on the minimum of $\mathcal{F}$. This implies that minimizers $\rho_0, \rho_\gamma \leq C\rho_{\rm fc}$, which gives the desired a priori upper bound on $\rho$.

*Step 4.* To finish the argument, we need to make more refined choices for both the upper and the lower bound. As an upper bound, we will use the minimum of the expression

$$\mathcal{F}_0(\gamma) - \mu\rho_\gamma + \widehat{V}(0)\rho_\gamma^2.$$

The minimizer will be the free gas minimizer $\gamma_{\delta_0}$ corresponding to a positive chemical potential $\delta_0 > 0$, determined such that $\rho_{\gamma_{\delta_0}} = (2\pi)^{-3}\int\gamma_{\delta_0}$ also minimizes

$$-\mu\rho_\gamma - \delta_0\rho_\gamma + \widehat{V}(0)\rho_\gamma^2,$$

i.e.

$$\mu + \delta_0 = 2\widehat{V}(0)\rho_{\gamma_{\delta_0}}.$$

Let us write

$$\delta_0 = \kappa^2\rho_{\rm fc}^{4/3}a^2$$

for some $\kappa$ that we will now determine. We know from (5.25) that the free gas minimizer $\gamma_{\delta_0}$ will have

$$\rho_{\gamma_{\delta_0}} = \rho_{\rm fc}(1 - C_2\kappa(\rho_{\rm fc}^{1/3}a + o(\rho_{\rm fc}^{1/3}a)))$$

for an appropriate constant $C_2 > 0$. Hence, the equation for $\kappa$ is

$$-2C_0\widehat{V}(0)\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a) + \kappa^2\rho_{\rm fc}^{4/3}a^2 = -2C_2\widehat{V}(0)\rho_{\rm fc}\kappa(\rho_{\rm fc}^{1/3}a + o(\rho_{\rm fc}^{1/3}a)),$$

that is,

$$\kappa^2 + 2C_2\kappa - 2C_0 = o(1), \tag{5.51}$$

where $C_0, C_2 > 0$.

We can use the a priori bounds in Proposition 19, and since we know that $\rho \leq C\rho_{\rm fc}$, we can express the error terms with $\rho$ replaced by $\rho_{\rm fc}$. We then go back to the expression (5.49) to get an improved lower bound. We set $t_0 = 0$ and only ignore the last double integral. We arrive at

$$\begin{aligned}\mathcal{F}(\gamma,\alpha,\rho_0) \quad &\geq \quad \mathcal{F}^{\rm S}(\gamma,\alpha,\rho_0) + (2\widehat{V}(0) - 8\pi a)\rho_0\rho_\gamma - \mu\rho \\ &\quad +4\pi a\rho_0^2 + \rho_\gamma^2\widehat{V}(0) - C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2},\end{aligned}$$

and apply Lemma 15 with

$$\delta = \delta_0 + (2\widehat{V}(0) - 8\pi a)\rho_0.$$

The expression for $G$ will then satisfy

$$\begin{aligned} G \quad &= \quad T^{-1}\sqrt{(p^2 + \delta_0 + (2\widehat{V}(0) - 8\pi a + \widehat{Vw}(p))\rho_0)^2 - \rho_0^2\widehat{Vw}(p)^2} \\ &\geq \quad T^{-1}\sqrt{((1 - C\rho_{\rm fc}a^3)p^2 + \delta_0) + 2\rho_0\widehat{V}(0))^2 - (8\pi a\rho_0)^2} \\ &\geq \quad T^{-1}\sqrt{((1 - C\rho_{\rm fc}a^3)p^2 + \delta_0)^2 + 4((1 - C\rho_{\rm fc}a^3)p^2 + \delta_0)\rho_0\widehat{V}(0)}.\end{aligned}$$

If we insert into the lower bound of Lemma 15 and bound the $G$-integral using Lemma 25 below, we obtain

$$\begin{aligned}
\mathcal{F}(\gamma,\alpha,\rho_0) &\geq \mathcal{F}_0(\gamma_{\delta_0}) + \delta_0\rho_{\gamma_{\delta_0}} + 2\rho_{\gamma_{\delta_0}}\widehat{V}(0)\rho_0 - C\rho_{\rm fc}^{2/3}(\rho_0 a)^{3/2} \\
&\quad -\delta_0\rho_\gamma - \mu\rho + 4\pi a\rho_0^2 + \rho_\gamma^2\widehat{V}(0) - C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2} \\
&\geq \mathcal{F}_0(\gamma_{\delta_0}) - \mu\rho_{\gamma_{\delta_0}} + \widehat{V}(0)\rho_{\gamma_{\delta_0}}^2 + (2\rho_{\gamma_{\delta_0}}\widehat{V}(0)-\mu)\rho_0 + 4\pi a\rho_0^2 \\
&\quad +\widehat{V}(0)(\rho_\gamma - \rho_{\gamma_{\delta_0}})^2 - C\rho_{\rm fc}^{2/3}(\rho_0 a)^{3/2} - C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2} \\
&= \mathcal{F}_0(\gamma_{\delta_0}) - \mu\rho_{\gamma_{\delta_0}} + \widehat{V}(0)\rho_{\gamma_{\delta_0}}^2 \\
&\quad +2(C_0 - C_2\kappa)\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)\rho_0\widehat{V}(0) + 4\pi a\rho_0^2 - C\rho_{\rm fc}^{2/3}(\rho_0 a)^{3/2} \\
&\quad +\widehat{V}(0)(\rho_\gamma - \rho_{\gamma_{\delta_0}})^2 - C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2} \\
&\geq \mathcal{F}_0(\gamma_{\delta_0}) - \mu\rho_{\gamma_{\delta_0}} + \widehat{V}(0)\rho_{\gamma_{\delta_0}}^2 \\
&\quad +2(C_0 - C_2\kappa)\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)\rho_0\widehat{V}(0) + 2\pi a\rho_0^2 - C\rho_{\rm fc}^2(\rho_{\rm fc}^{1/3}a)^2 \\
&\quad +\widehat{V}(0)(\rho_\gamma - \rho_{\gamma_{\delta_0}})^2 - C\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^{3/2}.
\end{aligned}$$

Thus we conclude, by choosing $C_0$ large enough (such that $C_0 - C_2\kappa$ will be positive), that

$$\rho_\gamma \leq \rho_{\gamma_{\delta_0}} + C\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{3/4}, \quad \rho_0 \leq C\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{3/4}.$$

We can now apply Proposition 21 and also the bound (5.42) to improve the last error term in the lines above. We consider the terms with the Laplacian in (5.40) and the second displayed estimate in Proposition 21 as error terms, which lead to an error of order $\rho_{\rm fc}^2 a(\rho_{\rm fc}^{1/3}a)^2$. We conclude that for $C_0$ large enough:

$$\rho_\gamma \leq \rho_{\gamma_{\delta_0}} + C\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a), \quad \rho_0 \leq C\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a).$$

We therefore find that

$$\rho \leq \rho_{\rm fc}(1 - C_0\kappa(\rho_{\rm fc}^{1/3}a + o(\rho_{\rm fc}^{1/3}a))) + C\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a).$$

By the expression for $\kappa$ it is therefore clear that by choosing $C_0$ large enough we obtain that

$$\rho \leq \rho_{\rm fc}(1 - C_1(\rho_{\rm fc}^{1/3}a))$$

as desired. The result obtained in step 1 and the reasoning in step 2 then finish the proof for temperatures $T \leq D\rho^{2/3}$.

*Step 5.* For $T > D\rho^{2/3}$, or equivalently, $\rho < D^{-3/2}T^{3/2}$, first note that the reasoning in step 1 without reference to Lemma 22 and Proposition 19 leads to an equivalent of (5.47) and the conclusion that there exists a constant $C_1$ such that $\rho_0 = 0$ for any minimizing triple with $\rho \leq \rho_{\rm fc} - C_1\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{1/2}$ satisfying the extra assumption that there is a $\mu$ that will give the same minimizer of the grand canonical problem. This is certainly sufficient for $\rho < D^{-3/2}T^{3/2}$, and we again try to employ the reasoning of step 2 to avoid the extra assumption. Luckily, it is immediately clear that $\rho_{0+} = 0$: either $\rho_+ \leq \rho_{\rm fc} - C_1\rho_{\rm fc}(\rho_{\rm fc}^{1/3}a)^{1/2}$, so that $\rho_{0+} = 0$, or the interval $[\rho_-, \rho_+]$ contains a density $\tilde\rho > D^{-3/2}T^{3/2}$, in which case the steps above imply that $\tilde\rho_{0+} = \rho_{0+} = 0$.

□

We have used the following lemma, which is proved in Appendix A.

**Lemma 25.** *For $0 \leq \delta_0, b \leq 1$ there exists a constant $C > 0$ such that*

$$\left| \int \ln\left(1 - e^{-\sqrt{(p^2+\delta_0)^2+2(p^2+\delta_0)b}}\right) dp - \int \ln(1 - e^{-(p^2+\delta_0)}dp - b\int (e^{p^2+\delta_0} - 1)^{-1} dp \right| \leq Cb^{3/2}.$$

5.6. **Preliminary approximations.** The previous sections have provided all the a priori knowledge we will need. In this section, we would like to approximate the integrals in Corollary 16 in different ways. The proof of all lemmas can be found in Appendix A.

We will be working with the general assumption (5.2) on $t_0$. We will also write $\delta = d\phi^2$, where $\phi$ will be chosen to be $\sqrt{\rho_0 a}$ or $Ta$ in later sections. Note that the dilute limit corresponds to $\phi \to 0$, so this is what we will assume throughout the section. To keep track of the different limits, we describe $\phi^2/T \ll 1$ as 'moderate temperatures', and $\phi^2/T \geq O(1)$ as 'low temperatures'. Also, a statement like '$\phi a \ll 1$' means $\phi a \leq C$ for some constant small enough.

We start by analysing the first contribution to the density in (5.18).

**Lemma 26** ($\rho_\gamma^{(1)}$ approximation)**.** *Let $\sigma_0 \geq 0$ and $d_0 \geq 0$ be fixed constants, and let $-1 \leq \theta \leq 0$, $0 \leq d \leq d_0$, $0 \leq \sigma \leq \sigma_0$, $\phi > 0$ and $0 \leq \rho_0 \leq \rho$. Assume $\rho_0 a/\phi^2 = \sigma/8\pi$ and let $\delta = d\phi^2$ and $t_0 = \theta\rho_0$. For $\phi a \ll 1$, we have*

$$\rho_\gamma^{(1)} = \phi^3 \frac{1}{2} I_3(d, \sigma, \theta) + o\left(\phi^3\right).$$

*The error is depends only on $\sigma_0$ and $d_0$.*

For the other contribution to $\rho_\gamma$, we need the following two results.

**Lemma 27** ($\rho_\gamma^{(2)}$ expansion for moderate temperatures)**.** *Let $\sigma_0 \geq 0$ and $d_0 \geq 0$ be fixed constants, and let $-1 \leq \theta \leq 0$, $0 \leq d \leq d_0$, $0 \leq \sigma \leq \sigma_0$, $\phi > 0$ and $0 \leq \rho_0 \leq \rho$. Assume $\rho_0 a/\phi^2 = \sigma/8\pi$ and let $\delta = d\phi^2$ and $t_0 = \theta\rho_0$. For $\phi^2/T \ll 1$, we have*

$$\begin{aligned}\rho_\gamma^{(2)} &= T^{3/2} I_4(d, \sigma, \theta, \phi/\sqrt{T}) + O\left(T^{5/2}a^2(\rho^{1/3}a)^{-3/8}\right) \\ &= \rho_{\text{fc}} - \frac{1}{8\pi}\left(\frac{\phi^2}{T}\right)^{1/2} T^{3/2}\left(\sqrt{d + 2(1+\theta)\sigma} + \sqrt{d}\right) \\ &\quad + o\left(T\phi\right) + O\left(T^{5/2}a^2(\rho^{1/3}a)^{-3/8}\right),\end{aligned}$$

*The error in the first line only depends on $\sigma_0$, the one in the second line on $\sigma_0$ and $d_0$.*

**Lemma 28** ($\rho_\gamma^{(2)}$ expansion for low temperatures)**.** *Let $0 \leq \rho_0 \leq \rho$, $d \geq 0$, $\sigma = 8\pi$ and $t_0 = \theta = 0$. Let $\delta = d\rho_0 a = d\phi^2$. Then, for $\phi a = \sqrt{\rho_0 a^3} \ll 1$ while $\phi^2/T = \rho_0 a/T \geq O(1)$, we have*

$$\rho_\gamma^{(2)} = T^{3/2} I_4(d, 8\pi, 0, \sqrt{\rho_0 a/T}) + o((\rho_0 a)^{3/2}).$$

*The error is uniform in $d \geq 0$ and $\rho_0$.*

A similar preliminary analysis can be done for the energy terms in Corollary 16.

**Lemma 29** ($F^{(1)}$ approximation). *Let $\sigma_0 \geq 0$ and $d_0 \geq 0$ be fixed constants, and let $-1 \leq \theta \leq 0$, $0 \leq d \leq d_0$, $0 \leq \sigma \leq \sigma_0$, $\phi > 0$ and $0 \leq \rho_0 \leq \rho$. Assume $\rho_0 a/\phi^2 = \sigma/8\pi$ and let $\delta = d\phi^2$ and $t_0 = \theta\rho_0$. For $\phi a \ll 1$, we have*

$$F^{(1)} = \phi^5 \frac{1}{2} I_1(d, \sigma, \theta) + o\left(\phi^5\right).$$

*The error is depends only on $\sigma_0$ and $d_0$.*

For the second term we will need the following two lemmas.

**Lemma 30** ($F^{(2)}$ expansion for moderate temperatures). *Let $\sigma_0 \geq 0$ and $d_0 \geq 0$ be fixed constants, and let $-1 \leq \theta \leq 0$, $0 \leq d \leq d_0$, $0 \leq \sigma \leq \sigma_0$, $\phi > 0$ and $0 \leq \rho_0 \leq \rho$. Assume $\rho_0 a/\phi^2 = \sigma/8\pi$ and let $\delta = d\phi^2$ and $t_0 = \theta\rho_0$. For $\phi^2/T \ll 1$, we have*

$$\begin{aligned} F^{(2)} &= T^{5/2} I_2(d, \sigma, \theta, \phi/\sqrt{T}) + O\left(T^{5/2}\phi^2 a^2 (\rho^{1/3}a)^{-1/4}\right) \\ &= T^{5/2} f_{\min} + \left(\frac{\phi^2}{T}\right) T\rho_{\mathrm{fc}}\left(d + (1+\theta)\sigma\right) \\ &\quad - \frac{1}{12\pi}\left(\frac{\phi^2}{T}\right)^{3/2} T^{5/2}\left((d + 2(1+\theta)\sigma)^{3/2} + d^{3/2}\right) \\ &\quad + o\left(T\phi^3\right) + O\left(T^{5/2}\phi^2 a^2 (\rho^{1/3}a)^{-1/4}\right). \end{aligned}$$

*The error in the first line only depends on $\sigma_0$, the one in the second line on $\sigma_0$ and $d_0$.*

**Lemma 31** ($F^{(2)}$ expansion for low temperatures). *Let $0 \leq \rho_0 \leq \rho$, $d \geq 0$, $\sigma = 8\pi$ and $t_0 = \theta = 0$. Let $\delta = d\rho_0 a = d\phi^2$. Then, for $\phi a = \sqrt{\rho_0 a^3} \ll 1$ while $\phi^2/T = \rho_0 a/T \geq O(1)$, we have*

$$F^{(2)} = T^{5/2} I_2(d, 8\pi, 0, \sqrt{\rho_0 a/T}) + o((\rho_0 a)^{5/2}).$$

*The error is uniform in $d \geq 0$ and $\rho_0$.*

We also prove two lemmas for the error terms (5.3) and (5.6) for minimizers of the form stated in Lemma 15.

**Lemma 32** (Error estimates for moderate temperatures). *Let $\sigma_0 \geq 0$ and $d_0 \geq 0$ be fixed constants, and let $-1 \leq \theta \leq 0$, $0 \leq d \leq d_0$, $0 \leq \sigma \leq \sigma_0$, $\phi > 0$ and $0 \leq \rho_0 \leq \rho$. Assume $\rho_0 a/\phi^2 = \sigma/8\pi$ and let $\delta = d\phi^2$ and $t_0 = \theta\rho_0$. For $\phi a \ll 1$, we have*

$$(E_2 + E_3)\left(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0\right) = O\left(Ta^3\rho\rho_0 + a\rho_0\phi^3\right),$$

*and*

$$E_4(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) = O(Ta^3\rho^2 + a\rho\phi^3).$$

*The error depends only on $\sigma_0$ and $d_0$.*

**Lemma 33** (Error estimates for low temperatures). *Let $d_0$ be a fixed constants, and let $0 \leq \rho_0 \leq \rho$, $0 \leq d \leq d_0$, $\sigma = 8\pi$ and $t_0 = \theta = 0$. Let $\delta = d\rho_0 a = d\phi^2$. Then, for $\phi a = \sqrt{\rho_0 a^3} \ll 1$ while $\rho a/T \geq O(1)$, we have*

$$(E_2 + E_3 + E_4)\left(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0\right) = o((\rho a)^{5/2}).$$

*The error is uniform in* $d \geq 0$.

We also prove a final lemma which will later be used to treat the error term $E_1$. Note that the reason we consider the function $f$ below is that $\alpha^{\rho_0,\delta} - \alpha_0 = -(2\pi)^3 t_0\delta_0 - f$.

**Lemma 34** (Preparation for estimates on $E_1$)**.** *Let* $\sigma_0 \geq 0$ *and* $d_0 \geq 0$ *be fixed constants, and let* $-1 \leq \theta \leq 0$, $0 \leq d \leq d_0$, $0 \leq \sigma \leq \sigma_0$, $\phi > 0$ *and* $0 \leq \rho_0 \leq \rho$. *Assume* $\rho_0 a/\phi^2 = \sigma/8\pi$, $\phi a \ll 1$, *and let* $\delta = d\phi^2$, $t_0 = \theta\rho_0$. *We define*

$$\begin{aligned} f(p) &:= (\rho_0 + t_0)\left(\frac{\beta(p)}{TG(p)} - \frac{1}{2p^2}\right)\widehat{Vw}(p). \\ &= \frac{1}{2}(\rho_0 + t_0)\widehat{Vw}(p)\left[\frac{1}{TG} - \frac{1}{p^2}\right] + \frac{(\rho_0 + t_0)\widehat{Vw}(p)}{TG(e^G - 1)}. \end{aligned} \tag{5.52}$$

*For* $\phi^2/T \ll 1$, *we have*

$$\int f(p)dp = T\phi(1+\theta)\sigma\frac{2\pi^2}{\sqrt{d + 2(1+\theta)\sigma} + \sqrt{d}} + o(T\phi),$$

*as well as*

$$\int |f(p)|dp \leq CT\phi \qquad \text{and} \qquad \int\limits_{|p|>\sqrt{T}} |f(p)|dp \leq C\phi^3.$$

*For* $\phi^2/T \geq O(1)$, *we have*

$$\int |f(p)|dp \leq C\phi^3.$$

*The errors above depend only on* $d_0$.

Note that some lemmas above assume that $d$ is bounded. In Subsections 5.7 and 5.8, we will argue that this can be assumed. For Subsection 5.8, we will need the following lemma to do this.

**Lemma 35.** *Let* $0 \leq \rho_0 \leq \rho$, $d \geq 0$, $\sigma = 8\pi$ *and* $t_0 = \theta = 0$. *Let* $\delta = d\rho_0 a = d\phi^2$. *For* $d \gg 1$, *we have*

$$F^{(1)} - d(\rho_0 a)\rho_\gamma^{(1)} \geq C\min\{d^{1/2}(\rho_0 a)^{5/2}, a^{-1}(\rho_0 a)^2\}.$$

*Also,* $\rho_\gamma^{(1)} \leq C(\rho_0 a)^{3/2}$ *and* $\rho_\gamma^{(1)} \to 0$ *as* $d \to \infty$.

The proof of all lemmas stated above can be found in Appendix A.

5.7. **Proof of Theorems 8 and 9.** According to the a priori estimate in Proposition 24, it suffices to zoom in on

$$|\rho - \rho_{\text{fc}}| < C\rho(\rho^{1/3}a) \tag{5.53}$$

within the region (4.1) to study the critical temperature: for larger $\rho$ there is a condensate, and for smaller $\rho$ there is none. Note that $\rho a/T \ll 1$ in this region, which was described as 'moderate temperatures' in the previous section. We actually have more a priori information: Lemma 22 states that $\rho_0$ is of order $\rho(\rho^{1/3}a)$, i.e. of order $T^2 a$.

For the non-interacting gas, the critical density is of order $T^{3/2}$. Since we are considering a weakly-interacting gas (through the dilute limit), one expects to again obtain an approximate critical density of order $T^{3/2}$. We therefore write

$$\rho = \rho_{\text{fc}} + \frac{k}{8\pi} T^2 a \tag{5.54}$$

for a dimensionless parameter $k$ (which is bounded in the region (5.53)). Note that $T^2 a = T^{3/2}(\sqrt{T}a) \ll T^{3/2}$, and so $T^2 a$ is indeed a lower order correction to $\rho_{\text{fc}}$. We also consider

$$\rho_0 = \frac{\sigma}{8\pi} T^2 a \qquad \phi = Ta \qquad \delta = dT^2 a^2 \tag{5.55}$$

for some dimensionless parameters $d \geq 0$ and $0 \leq \sigma \leq C$. It suffices to consider bounded $\sigma$ by Lemma 22. We will also show that the a priori estimates allow us to assume that $d$ is bounded. This gives access to the lemmas in the previous section since $\phi a = \phi^2/T = Ta^2 \ll 1$ in the dilute limit. Finally, we write

$$t_0 = \frac{\tau}{8\pi} T^2 a = \left(\frac{\tau}{\sigma}\right) \rho_0 = \theta \rho_0, \tag{5.56}$$

where $\tau = \theta\sigma \in \mathbb{R}$ is dimensionless.

We are free to choose $-\rho_0 \leq t_0 \leq 0$ depending on $\rho_0$ and $\delta$, as this was simply a parameter entering in Lemma 13 and the definition of $\alpha_0$ (see (5.4)). To be able to prove that the error term $E_1$ is indeed small for the $\alpha^{\rho_0,\delta}$ from Lemma 15, we will choose $t_0$ such that the self-consistent equation

$$\int (\alpha^{\rho_0,\delta} - \alpha_0) = 0 \tag{5.57}$$

is satisfied. The following lemma confirms that this choice implies that the error $E_1$ is small. It also shows that the equation above leads to a concrete equation for $\tau$ in terms of $\sigma \geq 0$ and $d \geq 0$, which implies that $-\sigma \leq \tau \leq 0$, i.e. $-1 \leq \theta \leq 0$.

**Lemma 36** (Self-consistent equation for $t_0$ and estimate on $E_1$)**.** *Under the assumptions introduced at the start of this subsection, in particular the self-consistent equation* (5.57) *and* $\sqrt{T}a \ll 1$*, we have*

$$\tau = -\frac{2(\sigma+\tau)}{\sqrt{d+2(\sigma+\tau)}+\sqrt{d}} + o(1). \tag{5.58}$$

*This equation has a unique solution for every* $d \geq 0$ *and* $\sigma \geq 0$*, and it satisfies* $-\sigma \leq \tau \leq 0$*. We also have*

$$\iint (\alpha^{\rho_0,\delta} - \alpha_0)(p)\widehat{V}(p-q)(\alpha^{\rho_0,\delta} - \alpha_0)(q)dpdq = o(T^4 a^3).$$

*The errors above holds uniformly in* $\sigma$ *and* $d$ *as long as they are bounded.*

*Proof. Step 1.* The self-consistent equation (5.57) says $(2\pi)^3 t_0 = -\int f$, with $f$ as in Lemma 34, so by using that lemma and the assumptions introduced at the start of this subsection, we conclude that (5.58) holds. To see that it always has a solution in $[-\sigma, 0]$, we rewrite the equation as

$$\tau\left(\sqrt{d+2(\sigma+\tau)}+\sqrt{d}\right) + 2(\sigma+\tau) = 0,$$

and note that the left-hand side is a continuous function which goes from $-2\sigma\sqrt{d} \leq 0$ to $2\sigma \geq 0$ as $\tau$ goes from $-\sigma$ to 0.
*Step 2.* We use Lemma 34 again to conclude that

$$\int |f(p)|dp \leq CT\phi = CT^2a, \qquad \int_{|p|>\sqrt{T}} |f(p)|dp \leq C\phi^3 = CT^3a^3.$$

Since $\alpha^{\rho_0,\delta} - \alpha_0 = -(2\pi)^3 t_0\delta_0 - f$ and $\int \alpha^{\rho_0,\delta} - \alpha_0 = 0$ by assumption, we have

$$\begin{aligned}
&\left|\int (\alpha^{\rho_0,\delta} - \alpha_0)(p)\widehat{V}(p-q)(\alpha^{\rho_0,\delta} - \alpha_0)(q)dpdq\right| \\
&= \left|\int (\alpha^{\rho_0,\delta} - \alpha_0)(p)\widehat{V}(p-q)(\alpha^{\rho_0,\delta} - \alpha_0)(q)dpdq - \widehat{V}(0)\left(\int \alpha^{\rho_0,\delta} - \alpha_0\right)^2\right| \\
&\leq 2(2\pi)^3|t_0|\int |\widehat{V}(p) - \widehat{V}(0)||f(p)|dp + \int |f(p)||\widehat{V}(p-q) - V(0)||f(q)|dpdq \\
&\leq C|t_0|T^3a^4 + CT^5a^5 = o(T^4a^3),
\end{aligned}$$

where we have used the fact that $|\widehat{V}(p) - \widehat{V}(0)| \leq Ca^3T$ for $|p| \leq \sqrt{T}$ and $|\widehat{V}(p)| \leq Ca$ for all $p$. □

Before we prove the main theorem, we state a final error estimate. Its proof can be found in Appendix A.

**Lemma 37** (Estimate on $E_5$)**.** *Under the assumptions introduced at the start of this subsection, in particular $\sqrt{T}a \ll 1$, we have*

$$E_5(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) = o(T^4a^3).$$

*This holds uniformly in $d$ and $\sigma$ as long as they are bounded.*

We are now ready to prove the first main theorem of the paper, which gives an expression for the critical temperature.

*Proof of Theorem 8.* We will work with the notation introduced at the start of this section. We again refer to Proposition 24, which contains the desired conclusion outside this region, so that we can restrict to the region (5.53). We also recall Lemma 22, which implies $\rho_0 \leq CT^2a$, so that we can consider $\sigma$ to be bounded.

The proof will proceed as follows. In step 1, we will calculate the simplified minimal energy as a function of $\rho$ and $\rho_0$. In step 2, we discuss the precise relation between the minimization problem of the simplified and canonical functionals. In step 3, we prove the theorem by minimizing the simplified energy in $0 \leq \rho_0 \leq \rho$.

*Step 1a.* We would like to calculate the simplified energy for $(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0)$. We assume that $t_0(\delta, \rho_0)$ is defined as in Lemma 36. Note that this means that $-1 \leq \theta \leq 0$ in (5.56), so that we can apply the lemmas from the previous subsection (although we have yet to establish boundedness of $d$ to obtain uniform errors in all cases, which we will do in step 1c.). Corollary

16 and Lemmas 29 and 30 together with (5.55) and (5.56) imply that for $\delta, \rho_0 \geq 0$:

$$\begin{aligned}\mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) &= \left(\mathcal{F}^{\mathrm{s}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) + \delta\rho_{\gamma^{\rho_0,\delta}}\right) - \delta\rho_{\gamma^{\rho_0,\delta}} \\ &\quad + \widehat{V}(0)\rho^2 + (12\pi a - \widehat{V}(0))\rho_0^2 - 8\pi a\rho\rho_0 - 4\pi a t_0^2 - 8\pi a t_0(\rho - \rho_0) \\ &= T^{5/2} f_{\min} - T^2 a^2(\rho - \rho_{\mathrm{fc}})(\sigma + \tau) + \widehat{V}(0)\rho^2 \\ &\quad + T^4 a^3 \Big[\frac{d}{8\pi}\left(\sqrt{d + 2(\sigma+\tau)} + \sqrt{d}\right) - \frac{(d + 2(\sigma+\tau))^{3/2} + d^{3/2}}{12\pi} \\ &\qquad + \frac{\tau\sigma}{8\pi} - \frac{\tau^2}{16\pi} + (12\pi - \nu)\frac{\sigma^2}{64\pi^2}\Big] + o\left(T^4 a^3\right),\end{aligned} \tag{5.59}$$

where we also used that according to Lemmas 26 and 27:

$$\rho_{\gamma^{\rho_0,\delta}} = \rho_{\mathrm{fc}} - \frac{T^2 a}{8\pi}\left(\sqrt{d + 2(\sigma+\tau)} + \sqrt{d}\right) + o(T^2 a). \tag{5.60}$$

The expressions above really only depend $d$ and $\sigma$, since $\tau$ satisfies (5.58). However, we are interested in rewriting the expression fully in terms of $\sigma$ and $k$. After all, we would like to investigate the nature of $\sigma$ (which defines $\rho_0$) for given $k$ (which defines $\rho$). First note that from the equation

$$\rho = \rho_0 + \rho_{\gamma^{\rho_0,\delta}} = \frac{\sigma}{8\pi} T^2 a + \rho_{\mathrm{fc}} - \frac{T^2 a}{8\pi}\left(\sqrt{d + 2(\sigma+\tau)} + \sqrt{d}\right) + o(T^2 a),$$

we obtain

$$\sqrt{d + 2(\sigma+\tau)} + \sqrt{d} = \sigma + 8\pi\frac{\rho_{\mathrm{fc}} - \rho}{T^2 a} = \sigma - k, \tag{5.61}$$

where $k$ is defined in (5.54). This yields

$$d = \left(\frac{(\sigma-k)^2 - 2(\sigma+\tau)}{2(\sigma-k)}\right)^2.$$

We can also rewrite $\tau$ in terms of $\sigma$ and $k$ by using (5.58) and (5.61):

$$\tau = \frac{2\sigma}{k - \sigma - 2} + o(1) \qquad \text{and} \qquad \sigma + \tau = \frac{\sigma(k-\sigma)}{k - \sigma - 2} + o(1). \tag{5.62}$$

We plug these expressions into (5.59) to obtain

$$\begin{aligned}\mathcal{F}^{\mathrm{sim}}(\gamma^{\rho,\rho_0}, \alpha^{\rho,\rho_0}, \rho_0) &= T^{5/2} f_{\min} + \widehat{V}(0)\rho^2 + T^4 a^3\left[\frac{1}{8\pi}\left(\frac{(\sigma-k)^3}{12}\right.\right. \\ &\quad \left.\left. -\sigma^2\Big(\frac{1}{2} + \frac{1}{2 + \sigma - k}\Big)\right) - (\nu - 8\pi)\frac{\sigma^2}{(8\pi)^2}\right] + o(T^4 a^3),\end{aligned} \tag{5.63}$$

where we now write $\gamma^{\rho_0,\rho}$ for the $\gamma^{\rho_0,\delta}$ that satisfies $\rho_{\gamma^{\rho_0,\delta}} + \rho_0 = \rho$. This can only be done for certain $\sigma$ and $k$: it was only for $\delta \geq 0$ that we were able to obtain minimizers of this form.

*Step 1b.* We now determine for which $\sigma$ and $k$ (5.63) holds. Using (5.61) and the equation for $\tau$ (5.58), we know that, given a $\rho_0 = \sigma\frac{T^2 a}{8\pi}$, minimizing the functional for some $d \geq 0$ leads to a minimizer with

$$\rho = \rho_{\mathrm{fc}} + \frac{T^2 a}{8\pi}\left(1 + \sigma - \sqrt{d} - \sqrt{1 + 2\sigma + d + 2\sqrt{d}}\right) + o(T^2 a),$$

The above expression is maximal for $d = 0$. Its value at this point is significant: fixing some $\rho_0$, we know that this is the maximal $\rho$ for which we will be able to find a minimizer to the simplified functional. This maximal $\rho$ is

$$\rho_{\max}(\sigma) = \rho_{\mathrm{fc}} + \frac{T^2 a}{8\pi} k_{\max}(\sigma) + o(T^2 a),$$

where we defined

$$k_{\max}(\sigma) = 1 + \sigma - \sqrt{1 + 2\sigma}.$$

Fixing some $k$, and considering all $\sigma \geq 0$, we can find out that (5.63) holds whenever

$$\sigma \in I(k) := \begin{cases} [0, \infty) & \text{if } k \leq 0 \\ \left[k + \sqrt{2k}, \infty\right) & \text{if } k > 0 \end{cases}. \tag{5.64}$$

Summarizing, it is for these $\sigma$ and $k$ that there exists a $(\gamma^{\rho_0,\rho}, \alpha^{\rho_0,\rho})$.

*Step 1c.* We will be interested in using (5.63) as a lower bound for the energy, where the error is uniform in $\sigma$ and $k$. We would now like to show that $d$ is bounded, so that we obtain uniform errors in (5.59), (5.60) and consequently (5.63).

As noted at the start of the proof, it suffices to consider $\rho_0 \leq CT^2 a$. Combined with (5.53), this tells us that $\rho_\gamma \geq \rho - C_0 T^2 a$ for some constant $C_0$. We claim that it suffices to restrict to $d \leq d_0$, which is chosen such that

$$\frac{2\sqrt{d_0}}{8\pi} \geq 2C_0.$$

To see this, consider $d > d_0$. Because $\rho_{\gamma^{\rho_0,\delta}}$ is decreasing in $\delta$ by the structure of the minimization problem in Lemma 15, we know that

$$\begin{aligned} \rho_{\gamma^{\rho_0,d}} \leq \rho_{\gamma^{\rho_0,d_0}} &= \rho_{\mathrm{fc}} - \frac{T^2 a}{8\pi}\left(\sqrt{d_0 + 2(\sigma + \tau)} + \sqrt{d_0}\right) + o(T^2 a) \\ &\leq \rho_{\mathrm{fc}} - 2C_0 T^2 a + o(T^2 a), \end{aligned}$$

where the error only depends on $d_0$ since we have a priori restricted to bounded $\sigma$. This violates the a priori restriction, confirming that we can restrict to $d \leq d_0$. We have obtained the important conclusion that we can think of the error in (5.63) as uniform.

*Step 2.* Our strategy will be to connect (5.63) to $\mathcal{F}^{\mathrm{can}}$ using Corollary 14. For convenience, we will first assume $k \leq 0$, so that all $0 \leq \sigma \in I(k)$.

On the one hand, any potential minimizer $(\gamma, \alpha, \rho_0)$ with $\rho_\gamma + \rho_0 = \rho$ will have to satisfy the a priori estimates in Propositions 21 and 23. This means that

$$\begin{aligned} &\mathcal{F}^{\mathrm{can}}(\gamma, \alpha, \rho_0) \\ &\geq \mathcal{F}^{\mathrm{sim}}(\gamma, \alpha, \rho_0) + \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3} \Delta\widehat{V}(0) T^4 - (E_2 + E_3 + E_5)(\gamma, \alpha, \rho_0) \\ &\geq \mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\rho}, \alpha^{\rho_0,\rho}, \rho_0) + \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3} \Delta\widehat{V}(0) T^4 - o(T^4 a^3). \end{aligned} \tag{5.65}$$

On the other hand, we have for any $\rho_0$:

$$\begin{aligned}
&\inf_{(\gamma,\alpha),\ \rho_0=\rho-\rho_\gamma} \mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) \leq \mathcal{F}^{\mathrm{can}}(\gamma^{\rho,\rho_0},\alpha^{\rho,\rho_0},\rho_0) \\
&\leq \mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\rho},\alpha^{\rho_0,\rho},\rho_0) + \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4 \\
&\qquad\qquad + (E_1+E_2+E_3+E_5)(\gamma^{\rho_0,\rho},\alpha^{\rho_0,\rho},\rho_0) \\
&\leq \mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\rho},\alpha^{\rho_0,\rho},\rho_0) + \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4 + o(T^4a^3),
\end{aligned} \tag{5.66}$$

where we have used Lemmas 32 and 36. The errors are uniform since we assume $d$ and $\sigma$ to be bounded.

We conclude that the energy of any potential minimizer matches (5.63) (up to the constant term and a small error). However, for any $\rho_0$ the expression (5.63) also provides an upper bound. Therefore, if we find that the minimizing $\sigma$ of (5.63) is non-zero, then the same should hold for the real minimizer. If the approximate minimizer is zero, we can only conclude that the real minimizer is approximately zero because of the small error. We will therefore need an extra step in this case

*Step 3a.* We now analyse (5.63) for given $k \leq 0$ and $\nu$ and find out whether its minimum $\sigma_{\min}$ is zero or not.

An analysis of (5.63) shows that there always is a single $k \leq 0$ where the character of the minimizer of changes (for given $\nu$)[1], which implies that a function $h_1(\nu)$ exists. We can also see that the critical $k$ decreases with $\nu$. For the limit $\nu \to 8\pi$, we numerically verify that the minimizing $\sigma_{\min}$ approximately satisfies

$$\sigma_{\min} = \begin{cases} 0 & \text{if } k < -1.28 \\ > 0 & \text{if } k > -1.28 \end{cases}. \tag{5.67}$$

This is illustrated by Figure 1 below, which shows (5.63) for three values of $k$.

Using the definition of $k$ (5.54), we conclude that the point where the nature of the minimizer changes is

$$\begin{aligned}
\rho_{\mathrm{c}} =& \rho_{\mathrm{fc}}\left(1 - \frac{1.28}{8\pi}\left(\frac{\zeta(3/2)}{8\pi^{3/2}}\right)^{-4/3}\rho_{\mathrm{fc}}^{1/3}a + o(\rho_{\mathrm{fc}}^{1/3}a)\right) \\
&\qquad\qquad = \rho_{\mathrm{fc}}\left(1 - 2.24\rho_{\mathrm{fc}}^{1/3}a + o(\rho_{\mathrm{fc}}^{1/3}a)\right).
\end{aligned}$$

We can also turn this into a criterion for the critical temperature. Given $\rho$ we know that the critical temperature $T_{\mathrm{c}}$ satisfies the equation above where $\rho_{\mathrm{fc}} = n_{\mathrm{fc}}T_{\mathrm{c}}^{3/2}$, where we calculated the constant $n_{\mathrm{fc}}$ in (5.21) (although it plays no role here). The free critical temperature would satisfy $\rho_{\mathrm{c}} = n_{\mathrm{fc}}T_{\mathrm{fc}}^{3/2}$.

[1]Because (5.63) depends on $\nu$ in an easy way, and is independent from $\nu$ for $\sigma = 0$, we can see that for every $k \leq 0$ there is a $\nu_0(k) \in [8\pi, \infty)$ such that $\sigma_{\min} > 0$ for $\nu > \nu_0(k)$. Moreover, $\nu_0(k)$ is continuous, monotone decreasing, and equal to $8\pi$ for $k = 0$. To reach the desired conclusion, we have to combine this with the following: for every $\nu \geq 8\pi$, there exists a $k$ negative enough such that $\sigma_{\min} = 0$. This can be seen by noting that the derivative in $\sigma$ it is positive for all $\sigma$ when $k$ is negative enough.

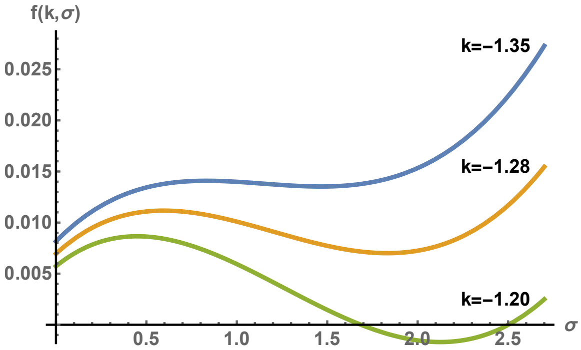


FIGURE 1. Plots of the part of the free energy that depends on $k$ and $\sigma$ (i.e. between the square brackets in (5.63), denoted by $f(k,\sigma)$ in the plot) for three values of $k$. For $k=-1.35$, $\sigma=\rho_0=0$ gives the lowest energy: no BEC. For $k=-1.20$, the minimum occurs at some $\rho_0>0$: BEC. The critical value is $k_c=-1.28$, where both $\sigma=0$ and $\sigma=1.83$ are minimizers.

Hence, we have

$$n_{\rm fc}T_{\rm fc}^{3/2}=n_{\rm fc}T_{\rm c}^{3/2}\left(1-2.24(\rho^{1/3}a)+o(\rho^{1/3}a)\right),$$

since we can write $\rho$ instead of $\rho_{\rm c}$ to leading order. In conclusion,

$$\begin{aligned}T_{\rm c}&=T_{\rm fc}\left(1-2.24(\rho^{1/3}a)+o(\rho^{1/3}a)\right)^{-2/3}\\&=T_{\rm fc}\left(1+1.49(\rho^{1/3}a)+o(\rho^{1/3}a)\right).\end{aligned}$$

*Step 3b.* For those values of $\rho$ where the minimizer of the approximate functional has $\rho_0=0$, we can only conclude that the exact minimizing $\rho_0$ is approximately zero. Because our energy approximation is accurate up to orders $T^4a^3$, we can only conclude $\rho_0=o(T^2a)$. We will need an extra argument to show that the energy increases for smaller $\rho_0$, which would then imply that the exact minimizer really is $\rho_0=0$.

Fixing $\rho$, first define

$$F_\rho(\rho_0)=\inf_{\int\gamma=\rho-\rho_0}\mathcal{F}^{\rm can}(\gamma,\alpha,\rho_0).$$

Note that it suffices to show there exists a $c_0>0$ such that

$$F_\rho(\rho_0)\geq F_\rho(0)+\frac{1}{2}c_0\rho_0T^2a^2(1-o(1))-2\rho_0^2\widehat{V}(0). \tag{5.68}$$

To prove this lower bound, we first minimize the terms in $\alpha$, and use Proposition 19:

$$\begin{aligned}\mathcal{F}^{\rm can}(\gamma,\alpha,\rho_0)\geq{}&\mathcal{F}^{\rm can}(\gamma,0,0)+2\widehat{V}(0)\rho_0\rho\\&-2\widehat{V}(0)\rho_0^2-c\rho_0T^2a^2(\sqrt{T}a)^{1/2}.\end{aligned}\tag{5.69}$$

To prove (5.68) from (5.69), we need to study

$$f_\rho(\rho_0)=\inf_{\int\gamma=\rho-\rho_0}\mathcal{F}^{\rm can}(\gamma,0,0)+2\rho_0\rho\widehat{V}(0),$$

which is convex in $\rho_0$.

We now use (5.65) and (5.66) to approximate the functional by $\mathcal{F}^{\text{sim}}$ and go back again, denoting the constant term as $C^{\text{sim}}T^4a^3$ and keeping in mind that the minimizer approximately has $\rho_0 = 0$ so that (5.65) does hold. We also apply (5.24), noting that $\rho_{\text{fc}} - \rho \geq 1.28T^2a$. For $\varepsilon > 0$, we find

$$\begin{aligned} f_\rho(-\varepsilon T^2 a) &\leq \inf_{\int \gamma = \rho + \varepsilon T^2 a} \mathcal{F}^{\text{sim}}(\gamma, 0, 0) - 2\varepsilon T^2 a \rho \widehat{V}(0) + C^{\text{sim}} T^4 a^3 + o(T^4 a^3) \\ &\leq \inf_{\int \gamma = \rho + \varepsilon T^2 a} \mathcal{F}_0(\gamma) + \widehat{V}(0)\rho^2 + c\varepsilon^2 T^4 a^3 + C^{\text{sim}} T^4 a^3 + o(T^4 a^3) \\ &\leq \inf_{\int \gamma = \rho} \mathcal{F}_0(\gamma) - (c_0\varepsilon - c\varepsilon^2) T^4 a^3 + \widehat{V}(0)\rho^2 + C^{\text{sim}} T^4 a^3 + o(T^4 a^3) \\ &\leq f_\rho(0) - (c_0\varepsilon - c\varepsilon^2) T^4 a^3 + o(T^4 a^3). \end{aligned}$$

We therefore conclude that there exists an $\varepsilon_0$ small enough such that

$$f_\rho(-\varepsilon_0 T^2 a) \leq f_\rho(0) + \frac{1}{2} c_0 (-\varepsilon_0 T^2 a) T^2 a^2.$$

Convexity of $f_\rho$ now implies that for $\rho_0 \geq 0$

$$f_\rho(\rho_0) \geq f_\rho(0) + \frac{1}{2} c_0 \rho_0 T^2 a^2.$$

This, as well as taking the infimum over $\gamma$ with $\int \gamma = \rho - \rho_0$ in (5.69), now gives the desired lower bound (5.68).

*Step 3c.* The theorem is still not quite proved, as we still have to show that the minimizing $\sigma$ is strictly positive for $k > 0$, which corresponds to $\rho > \rho_{\text{fc}}$. For $\sigma = 0$, we cannot use the simplified energy (5.63) because of the problem discussed in step 1b, but we can still use the first step in the lower bound (5.65): if the minimum occurs at $\rho_0 = 0$, we know that

$$\begin{aligned} &\inf_{(\gamma,\alpha),\ \rho_\gamma = \rho} \mathcal{F}^{\text{can}}(\gamma, \alpha, 0) - \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3} \Delta \widehat{V}(0) T^4 \\ &\quad \geq \inf_{(\gamma,\alpha),\ \rho_\gamma = \rho} \mathcal{F}^{\text{sim}}(\gamma, \alpha, 0) + o(T^4 a^3) = T^{5/2} f_{\min} + \widehat{V}(0)\rho^2 - o(T^4 a^3), \end{aligned}$$

where $t_0 = 0$ for $\rho_0 = 0$ (which is consistent with (5.62)). Since (5.63) holds at $\sigma = k + \sqrt{2k} \in I(k)$, we can see that it has a simplified energy of

$$T^{5/2} f_{\min} + \widehat{V}(0)\rho^2 + T^4 a^3 \left[ -\frac{k\left(3\sqrt{2}k^{3/2} + 20k + 23\sqrt{2}\sqrt{k} + 18\right)}{24\pi\left(\sqrt{2}\sqrt{k} + 2\right)} \right],$$

which is lower than the value at $\sigma = 0$. Using the upper bound (5.66), we conclude that the minimizer cannot have $\rho_0 = 0$ when $\rho > \rho_{\text{fc}}$. □

*Proof of Theorem 9. Step 1.* We now turn to the grand-canonical problem. That means that we should analyse the structure of minimizers of

$$\inf_{\rho \geq 0} \left[ \inf_{(\gamma,\alpha,\rho_0),\ \rho_\gamma + \rho_0 = \rho} \mathcal{F}^{\text{can}}(\gamma, \alpha, \rho_0) - \mu\rho \right] \tag{5.70}$$

for given $\mu \in \mathbb{R}$. This requires that we calculate the canonical free energy for any given $\rho$, but we note that it again suffices to only calculate it for (5.53), i.e. $|\rho - \rho_{\text{fc}}| < C\rho(\rho^{1/3}a)$. By the a priori result from Proposition 24, we know that if minimizer has a smaller $\rho$, it has $\rho_0 = 0$, and if it has a bigger $\rho$, it has $\rho_0 > 0$. Since the minimizing $\rho$ increases with $\mu$, this fits with the statement of the theorem.

In the region around the critical temperature, it seems natural to use the bounds (5.65) and (5.66) and simply minimize (5.63), but we only have these bounds for $\sigma \in I(k)$ (see (5.62) and (5.64)). In fact, the simplified functional has so far only been defined in this region as we have only made a choice for $t_0$ for $\delta, \rho_0 \geq 0$. To solve this problem, we now define

$$\tau(k,\sigma) = 1 - \sqrt{1+2\sigma}$$

for $\sigma \in [0,\infty)\backslash I(k)$, which is chosen because it is the value obtained for $\delta = 0$. In the spirit of (5.65), we know that any potential minimizer should satisfy

$$\begin{aligned}
&\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) - \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4 \\
&\geq \mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,\rho_0) - (E_2+E_3+E_5)(\gamma,\alpha,\rho_0) \\
&\geq \inf_{(\gamma,\alpha)} \mathcal{F}^{\mathrm{s}}(\gamma,\alpha,\rho_0) + \widehat{V}(0)\rho^2 - o(T^4a^3) \\
&\qquad\qquad + (12\pi a - \widehat{V}(0))\rho_0^2 - 8\pi a\rho\rho_0 - 4\pi a t_0^2 - 8\pi a t_0(\rho-\rho_0) \\
&= T^{5/2} f_{\min} + \widehat{V}(0)\rho^2 + T^4a^3\Big[ -(\sigma+\tau)\frac{k}{8\pi} - \frac{1}{12\pi}(2\sigma+2\tau)^{3/2} \\
&\qquad\qquad + (12\pi-\nu)\left(\frac{\sigma}{8\pi}\right)^2 - 4\pi\left(\frac{\tau}{8\pi}\right)^2 + \frac{\tau\sigma}{8\pi}\Big] - o(T^4a^3),
\end{aligned}$$

where we have used that the infimum of $\mathcal{F}^{\mathrm{s}}$ is attained at $(\gamma^{\rho_0,\delta=0}, \alpha^{\rho_0,\delta=0})$, with an energy given by (5.59). Minimizing this lower bound over $[0,\infty)\backslash I(k)$, we find that the infimum is attained at the boundary, i.e. at $\sigma = k + \sqrt{2k}$. Since the lower bound matches (5.63) at this point, we conclude that the minimizer of the canonical free energy has $\sigma \in I(k)$, so that it suffices to minimize (5.70) over $I(k)$ by the upper and lower bounds (5.65) and (5.66).

*Step 2.* Making the result of the previous step explicit, we now know that for $|\rho - \rho_{\mathrm{fc}}| < C\rho(\rho^{1/3}a)$:

$$\begin{aligned}
&\inf_{(\gamma,\alpha,\rho_0),\ \rho_\gamma+\rho_0=\rho} \mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0) - \mu\rho \\
&= T^{5/2} f_{\min} + \widehat{V}(0)\rho_{\mathrm{fc}}^2 - \mu\rho_{\mathrm{fc}} + T^2a^2\left(2\left(\frac{\nu}{8\pi}\right)\rho_{\mathrm{fc}} - \frac{\mu}{8\pi a}\right)k \\
&\quad + T^4a^3 \inf_{\sigma\in I(k)}\Big[\frac{1}{8\pi}\left(\frac{(\sigma-k)^3}{12} - \sigma^2\Big(\frac{1}{2} + \frac{1}{2+\sigma-k}\Big)\right) \\
&\qquad\qquad\qquad\qquad - (\nu-8\pi)\frac{\sigma^2}{(8\pi)^2} + \nu\frac{k^2}{(8\pi)^2}\Big] \\
&\quad + \frac{\zeta(3/2)\zeta(5/2)}{256\pi^3}\Delta\widehat{V}(0)T^4 + o\left(T^4a^3\right).
\end{aligned}$$

To consider the case $\nu \to 8\pi$, we show a plot of the function

$$g(k) = \inf_{\sigma\in I(k)}\Big[\frac{1}{8\pi}\left(\frac{(\sigma-k)^3}{12} - \sigma^2\Big(\frac{1}{2}+\frac{1}{2+\sigma-k}\Big)\right) + \frac{k^2}{8\pi}\Big] + 0.226k. \tag{5.71}$$

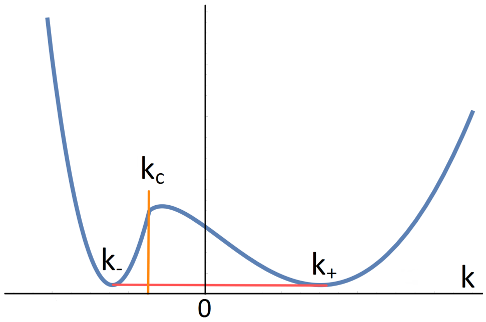


FIGURE 2. The curve shows the energy function $g(k)$ in (5.71). The two minima are $k_- = -2.23$ and $k_+ = 3.04$, and the critical value (shown in orange) is $k_c = -1.28$, which corresponds to the value of $k$ where $\sigma$ jumps to a positive value (see (5.67)). The derivative has a discontinuity at this point. The energy curve is not convex; the red line indicates the convex hull of the curve.

in Figure 2. Here, the value 0.226 was chosen such that the convex hull is obtained by replacing the curve between two minima by a constant function.

The two minima are

$$k_- = -2.23, \quad k_+ = 3.04$$

and the value here is $g(k_\pm) = -0.27$. Hence we have a first-order phase transition where the density jumps between the critical values corresponding to $k_\pm$. This conclusion is unaltered by the fact that we can only determine the energy curve up to a small error.

Note that the minimizer changes from $\rho_0 = 0$ to $\rho_0 > 0$ at the jump since $k_- \leq -1.28 \leq k_+$. We conclude that the critical chemical potential in the limit $\nu \to 8\pi$ is given by

$$\begin{aligned}\frac{\mu_c}{8\pi} &= 2\rho_{fc}a - 0.226T^2a^2 + o(T^2a^2) \\ &= \frac{1}{8\pi}\frac{2\zeta(3/2)}{\sqrt{\pi}}T^{3/2}a\left(1 - 0.226 \cdot 8\pi\frac{\sqrt{\pi}}{2\zeta(3/2)}\sqrt{T}a + o(\sqrt{T}a)\right).\end{aligned}$$

This can also be inverted to yield the critical temperature for $\mu > 0$:

$$\begin{aligned}T_c &= \left(\frac{\sqrt{\pi}}{2\zeta(3/2)}\right)^{2/3}\left(\frac{\mu}{a}\right)^{2/3} + \frac{2}{3}\cdot 0.226 \cdot 8\pi\left(\frac{\sqrt{\pi}}{2\zeta(3/2)}\right)^2 \mu + o(\mu) \\ &= \left(\frac{\sqrt{\pi}}{2\zeta(3/2)}\right)^{2/3}\left(\frac{\mu}{a}\right)^{2/3} + 0.44\mu + o(\mu),\end{aligned}$$

where the expansion is correct for $\mu \geq 0$ corresponding to $\rho^{1/3}a \ll 1$. An analysis for general $\nu$ (in which case the leading term of $\mu_c$ has an extra factor $\nu/8\pi$), combined with the existence of the function $h_1(\nu)$ from the previous theorem, allows the reader to deduce the existence of $h_2(\nu)$. □

*Remark* 38. Note that the existence of two minima shows that the grand canonical functional in general will not have a unique minimizer. As for the canonical case: we have coexistence of the two minimizers (one with $\rho_0 = 0$

and one with $\rho_0 > 0$) for $\rho$ between the two values defined by $k_\pm$. This means that at least part of the gas has a condensate for any $k \in [k_-, k_+]$. Hence one could say that (part of) the system is in a condensed phase from $k_-$ onwards.

5.8. **Proof of Theorems 10 and 11.** In this section, we simply set $t_0 = 0$. We will write $\delta = d\rho_0 a = d\phi^2$, with $d \geq 0$. Note that this implies that $\sigma = 8\pi$ in the lemmas of Subsection 5.6.

*Remark* 39 (Properties of the integrals)*.* We will use the following properties of the integrals (4.5) with $d, s \geq 0$:

- $I_1(d, 8\pi, 0) - dI_3(d, 8\pi, 0)$ monotonically increases to infinity in $d$.
- $I_2(d, 8\pi, 0, s) - ds^2 I_4(d, 8\pi, 0, s)$ monotonically increases to 0 in both $d$ and $s$ and it is bounded.
- $I_2(d, 8\pi, 0, s)$ monotonically increases to 0 in both $d$ and $s$ and it is bounded.
- $I_4(d, 8\pi, 0, s)$ monotonically decreases to zero in both $d$ and $s$ and it is bounded.

*Proof of Theorems 10 and 11.* Throughout the proof, we will distinguish between the regions $\rho a/T \ll 1$ ('moderate temperatures') and $\rho a/T \geq O(1)$ ('low temperatures'). For simplicity, we aim to write statements with a uniform error $o(T(\rho a)^{3/2} + (\rho a)^{5/2})$, i.e. $o(T(\rho a)^{3/2})$ in the first region, and $o((\rho a)^{5/2})$ in the second. Note that an error of $O((\rho a)^{5/2})$ satisfies this for $\rho a/T \ll 1$.

*Step 1a.* As in Subsection 5.7, we consider upper and lower bounds. First assume that $\delta \geq 0$ and $\rho_0 \geq 0$ are such that

$$\rho = \rho_0 + \rho_{\gamma^{\rho_0,\delta}}. \tag{5.72}$$

Similar to before, this may not always have a solution for given $\rho$ and $\rho_0$. By Lemma 13 and the a priori estimates in Proposition 19, we then know that any potential minimizer has to satisfy

$$\begin{aligned}\mathcal{F}^{\text{can}}(\gamma, \alpha, \rho_0) &\geq \mathcal{F}^{\text{sim}}(\gamma, \alpha, \rho_0) - (E_2 + E_3 + E_4)(\gamma, \alpha, \rho_0) \\ &\geq \mathcal{F}^{\text{sim}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) - O((\rho a)^{5/2}).\end{aligned} \tag{5.73}$$

Using Lemma 32 for $\rho a/T \ll 1$, Lemma 33 for $\rho a/T \geq O(1)$, and Lemma 34 for both, we find that[2]

$$\begin{aligned}&\inf_{(\gamma,\alpha),\ \rho_0=\rho-\rho_\gamma} \mathcal{F}^{\text{can}}(\gamma, \alpha, \rho_0) \leq \mathcal{F}^{\text{can}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) \\ &\leq \mathcal{F}^{\text{sim}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) + (E_1 + E_2 + E_3 + E_4)(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) \\ &\leq \mathcal{F}^{\text{sim}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) + o(T(\rho a)^{3/2} + (\rho a)^{5/2}).\end{aligned} \tag{5.74}$$

It is important to realize that we have yet to establish uniformity of the error in the upper bound, whereas the error in the lower bound is uniform.

[2]To obtain the estimate on $E_1$, we use $|\int(\alpha - \alpha_0)\widehat{V}(\alpha - \alpha_0)| \leq \widehat{V}(0)(\int|\alpha - \alpha_0|)^2$ and the fact that $|\alpha^{\rho_0,\delta} - \alpha_0|$ is equal to the $|f|$ in the statement of Lemma 34 since $t_0 = 0$.

*Step 1b.* The first line of the lower bound (5.73) allows us to prove the desired conclusion for $T > T_{\mathrm{fc}}\left(1 + h_1(\nu)\rho^{1/3}a + o(\rho^{1/3}a)\right)$. After all, Theorem 8 tells us that the minimizer has $\rho_0 = 0$ in this region, so that we find that

$$F^{\mathrm{can}}(T,\rho) \geq \inf_{(\gamma,\alpha),\ \rho=\rho_\gamma} \mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,0) = F_0(T,\rho) + \widehat{V}(0)\rho^2 - O((\rho a)^{5/2}),$$

where $F_0(T,\rho)$ is the free energy (5.20) of the non-interacting gas. We now note that

$$\inf_{(\gamma,\alpha)} \mathcal{F}^{\mathrm{can}}(\gamma,\alpha,0) = \inf_{\gamma} \mathcal{F}^{\mathrm{can}}(\gamma,0,0) \leq \inf_{\gamma} \mathcal{F}^{\mathrm{sim}}(\gamma,0,0),$$

which proves the result in this region.

*Step 2.* Using Lemma 31 and the first line of Lemma 30, we have

$$\begin{aligned}\mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\delta},\alpha^{\rho_0,\delta},\rho_0) = {} & F^{(1)} + T^{5/2} I_2(d, 8\pi, 0, \sqrt{\rho_0 a/T}) \\ & - d\rho_0 a(\rho-\rho_0) \\ & + \widehat{V}(0)\rho^2 - 8\pi a\rho_0\rho + \rho_0^2(12\pi a - \widehat{V}(0)) \\ & + o\left(T(\rho a)^{3/2} + (\rho a)^{5/2}\right),\end{aligned} \tag{5.75}$$

together with

$$\rho_{\gamma^{\rho_0,\delta}} = \rho_\gamma^{(1)} + T^{3/2} I_4(d, 8\pi, 0, \sqrt{\rho_0 a/T}) + o\left(T(\rho a)^{1/2} + (\rho a)^{3/2}\right). \tag{5.76}$$

In the last line, we have used Lemma 28 and the first line of Lemma 27. To use these lemmas, we have distinguished two cases: $\rho a/T \ll 1$, which implies $\rho_0 a/T = \phi^2/T \ll 1$; and $\rho a/T \geq O(1)$, which implies $\rho_0 a/T \geq O(1)$ by the a priori estimate (5.35). Note that the errors in the two equations above are uniform in $d$.

We know that $\rho_{\gamma^{\rho_0,\delta}}$ is decreasing in $\delta = d\rho_0 a$ by the structure of the minimization problem in Lemma 15. In fact, Lemma 35 and the fourth property in Remark 39 show that $\rho_{\gamma^{\rho_0,\delta}}$ decreases to 0 as $d \to \infty$. We therefore have that the equation (5.72) has a solution for every $\rho_0$ and $\rho$ such that

$$\rho - \rho_{\gamma^{\rho_0,\delta=0}} \leq \rho_0 \leq \rho, \tag{5.77}$$

or, denoting the solution to (5.76) for given $\rho$ and $d \geq 0$ by $\rho_0(d)$, for every $\rho_0(d=0) \leq \rho_0 \leq \rho$. Our assumption (5.72) amounts to plugging $\rho_0(d)$ into the simplified energy (5.75). In the next step, we do this for the different regions.

*Step 3: $\rho a/T \ll 1$.* In this step, we prove Theorem 11.

*Step 3a.* In order to be able to use more of the lemmas from Subsection 5.6, we need to show that we can assume that $d$ is bounded. We use (5.73), (5.75) and Lemma 35 to see that for $d \gg 1$ and $s = \sqrt{\rho_0 a/T}$:

$$\begin{aligned}\mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\delta},\alpha^{\rho_0,\delta},\rho_0) \geq {} & 4\pi a\rho^2 + T^{5/2}(I_2(d,8\pi,0,s) - ds^2 I_4(d,8\pi,0,s)) \\ & + 2(\nu - 8\pi)\rho a T^{3/2} I_4(d,8\pi,0,s) \\ & + (12\pi - \nu)a(T^{3/2} I_4(d,8\pi,0,s))^2 - o(T(\rho a)^{3/2})\end{aligned}$$

with errors uniform in $d$. As $d$ increases, $s$ increases, and this expression gets exponentially close to $4\pi a\rho^2$ as $d \to \infty$, and thus it is higher than the value provided by the upper bound 5.74 for $d = 0$ (see (5.79) for a calculation). We can therefore restrict to bounded $d$.

*Step 3b.* We conclude that the upper bound (5.74) has an error uniform in $d$. We can also apply Lemmas 26, 27, 29 and 30 to (5.75) to obtain

$$\begin{aligned}\mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0,\delta},\alpha^{\rho_0,\delta},\rho_0) &= T^{5/2}f_{\min} + \left(\frac{\rho_0(d)a}{T}\right)T\rho_{\mathrm{fc}}(d+8\pi)\\ &\quad - \frac{1}{12\pi}\left(\frac{\rho_0(d)a}{T}\right)^{3/2}T^{5/2}\left((d+16\pi)^{3/2}+d^{3/2}\right)\\ &\quad - d\rho_0(d)a(\rho-\rho_0(d)) + \widehat{V}(0)\rho^2 - 8\pi a\rho_0(d)\rho + \rho_0(d)^2(12\pi a - \widehat{V}(0))\\ &\quad + o(T(\rho a)^{3/2}),\end{aligned}$$

where

$$\rho_0(d) = \rho - \rho_{\mathrm{fc}} + \frac{1}{8\pi}\left(\frac{\rho_0(d)a}{T}\right)^{1/2}T^{3/2}\left(\sqrt{d+16\pi}+\sqrt{d}\right) + o(T(\rho a)^{1/2}), \tag{5.78}$$

and the errors are uniform in $d$. We conclude that $\rho_0 = \rho - \rho_{\mathrm{fc}} =: \Delta\rho$ to leading order. Rewriting the expansion in the small parameter $\Delta\rho a/T$, we obtain

$$\begin{aligned}&\mathcal{F}^{\mathrm{sim}}(\gamma^{\rho_0(d),\delta},\alpha^{\rho_0(d),\delta},\rho_0(d))\\ &= T^{5/2}f_{\min} + 4\pi a\rho^2 + (\widehat{V}(0)-4\pi a)\rho_{\mathrm{fc}}(2\rho-\rho_{\mathrm{fc}})\\ &\quad + T(\Delta\rho a)^{3/2}\left(\frac{1}{24\pi}\right)\left[(\sqrt{d+16\pi}+\sqrt{d})(d+6(8\pi-\nu)) - 32\pi\sqrt{d+16\pi}\right]\\ &\quad + o\left(T(\rho a)^{3/2}\right).\end{aligned} \tag{5.79}$$

This can explicitly be minimized in $d \geq 0$. The minimum is obtained for $d = 2(\nu - 8\pi)$, which leads to the expression stated in Theorem 11.

*Step 3c.* The proof is unfinished since the upper and lower bounds (5.73) and (5.74) only hold for $\rho_0$ satisfying (5.77), i.e. $\rho_0(d=0) \leq \rho_0 \leq \rho$. We need to deal with all other $\rho_0$ as we did in step 1 of the proof of Theorem 9: by revising the lower bound (5.73). We know that any potential minimizer should satisfy

$$\begin{aligned}&\mathcal{F}^{\mathrm{can}}(\gamma,\alpha,\rho_0)\\ &\geq \mathcal{F}^{\mathrm{sim}}(\gamma,\alpha,\rho_0) - (E_2+E_3+E_4)(\gamma,\alpha,\rho_0)\\ &\geq \inf_{(\gamma,\alpha)}\mathcal{F}^{\mathrm{s}}(\gamma,\alpha,\rho_0) + \widehat{V}(0)\rho^2 - 8\pi a\rho\rho_0 + (12\pi a - \widehat{V}(0))\rho_0^2 - O((\rho a)^{5/2})\\ &= T^{5/2}f_{\min} + 8\pi a\rho_0\rho_{\mathrm{fc}} - \left(\frac{\rho_0 a}{T}\right)^{3/2}T^{5/2}\frac{4}{3}\sqrt{16\pi}\\ &\qquad\qquad + \widehat{V}(0)\rho^2 - 8\pi a\rho_0\rho + \rho_0^2(12\pi a - \widehat{V}(0)) - o(T(\rho a)^{3/2}),\end{aligned} \tag{5.80}$$

where we have used the energy expansion (5.75) and Lemma 30 for the unrestricted minimizer $(\gamma^{\rho_0,\delta=0},\alpha^{\rho_0,\delta=0})$. Using $\nu \geq 8\pi$, we see that lower bound has a negative derivative for

$$0 \leq \rho_0 \leq \Delta\rho + \left(\frac{\Delta\rho a}{T}\right)^{1/2} T^{3/2}\frac{1}{\sqrt{\pi}} + o(T(\rho a)^{1/2}),$$

which is indeed bigger than

$$\rho_0(d=0) = \Delta\rho + \left(\frac{\Delta\rho a}{T}\right)^{1/2} T^{3/2}\frac{1}{2\sqrt{\pi}} + o(T(\rho a)^{1/2}).$$

Since this lower bound matches our earlier lower bound (5.79) at this point and the upper bound (5.74) also holds at this point, we can conclude that it suffices to consider the infimum over $\rho_0(d=0) \leq \rho_0 \leq \rho$, which yielded the desired result in step 3b, and proves Theorem 11.

*Step 4: $\rho a/T \geq O(1)$.* In this step, we make further preparations for the proof of Theorem 10.

*Step 4a.* To prove that we can assume that $d$ is bounded, we use (5.73), (5.75), boundedness of $I_2$ and $I_4$, and Lemma 35 to see that for $d \gg 1$:

$$\begin{aligned}\mathcal{F}^{\text{sim}}(\gamma^{\rho_0,\delta}, \alpha^{\rho_0,\delta}, \rho_0) &\geq 4\pi a\rho^2 + F^{(1)} - d(\rho_0 a)\rho_\gamma^{(1)} - O((\rho a)^{5/2}) \\ &\geq 4\pi a\rho^2 + C\min\{(\rho_0 a)^{5/2} d^{1/2}, a^{-1}(\rho_0 a)^2\} - O((\rho a)^{5/2}).\end{aligned}$$

with errors uniform in $d$. For $d \gg 1$, this is of higher order than $4\pi a\rho^2 + O((\rho a)^{5/2})$, which is the value provided by the upper bound (5.74) at $d = 0$. We can therefore restrict to bounded $d$.

*Step 4b.* We again need to establish that it suffices to minimize (5.75) over $d \geq 0$, i.e. to exclude $0 \leq \rho_0 \leq \rho_0(d=0)$ as potential minimizers. To do this, we repeat the lower bound (5.80). For $\rho a/T \geq O(1)$, the infimum of $\mathcal{F}^{\text{s}}$ is $O((\rho a)^{5/2})$ by Lemmas 26 and 29 and boundedness of $I_2$ and $I_4$. We obtain

$$\mathcal{F}^{\text{can}}(\gamma, \alpha, \rho_0) \geq \widehat{V}(0)\rho^2 + (12\pi a - \widehat{V}(0))\rho_0^2 - 8\pi a\rho\rho_0 - O((\rho a)^{5/2}).$$

Using $\nu \geq 8\pi$, we see that this has a negative derivative throughout the region, and as such the minimum can be found at the boundary (up to a lower order error), where it matches the lower bound (5.73) and the upper bound (5.74), and so we conclude that it suffices to consider the infimum over $\rho_0(d=0) \leq \rho_0 \leq \rho$.

*Step 4c.* We would now like to show that the errors in the lower bound (5.73) are $o((\rho a)^{5/2})$, rather than $O((\rho a)^{5/2})$. The above conclusion, Lemma 26 and the lower and upper bounds (5.73) and (5.74) imply that any potential minimizer has to satisfy

$$\rho_\gamma \leq \rho - \rho_0(d=0) = O((\rho a)^{3/2}).$$

We can now use this to improve the a priori bounds in Proposition 19, and hence lower the error in the lower bound (5.73) to $o((\rho a)^{5/2})$: we simply repeat the estimates (5.31), (5.32) and (5.33), and notice that we are able to pick a better $b$ because we know that $\rho_\gamma$ is small.

*Step 5.* Combining the steps above, we conclude

$$\begin{aligned}F^{\mathrm{can}}(T,\rho) = \inf_{0\le d\le d_0} [\frac{1}{2}(\rho_0(d)a)^{5/2} I_1(d,8\pi,0) + T^{5/2} I_2(d,8\pi,0,\sqrt{\rho_0(d)a/T})\\ - d\rho_0(d)a(\rho-\rho_0(d))\\ + \widehat{V}(0)\rho^2 - 8\pi a\rho_0(d)\rho + \rho_0(d)^2(12\pi a - \widehat{V}(0))]\\ + o\left((\rho a)^{5/2} + T(\rho a)^{3/2}\right),\end{aligned}$$

where

$$\rho_0(d) := \rho - \frac{1}{2}(\rho_0(d)a)^{3/2} I_3(d,8\pi,0) - T^{3/2} I_4(d,8\pi,0,\sqrt{\rho_0(d)a/T}).$$

Here, the errors in $\rho_0(d)$ have been dropped compared to (5.76) since they can be absorbed in the errors in the energy expression.

To finish the proof of Theorem 10, we just have to make a few replacements in the minimization problem above. These are

- replacing $(\rho_0 a)^{5/2} I_1(d,8\pi,0)$ by $(\rho a)^{5/2} I_1(d,8\pi,0)$. The error made is $O((\rho a)^{5/2})$ for $\rho a/T \ll 1$, which is acceptable. For $\rho a/T \ge O(1)$, we have $\rho_0(d) = \rho$ to leading order, so we make an error of $o((\rho a)^{5/2})$.
- replacing the similar term in $\rho_0(d)$. This is done in a similar way. We absorb the error in the energy expansion.
- replacing $T^{3/2} I_4(d,8\pi,0,\sqrt{\rho_0(d)a/T})$ by $T^{3/2} I_4(d,8\pi,0,\sqrt{\Delta\rho a/T})$. For $\rho a/T \ll 1$, we use (5.78) to see that this leads to an error that can be absorbed in the energy expansion. For $\rho a/T \ge O(1)$, this term is $O((\rho a)^{3/2})$ and $\rho_0(d) = \rho$ to leading order, so that the error is of lower order and the replacement is justified.

□

*Comment about Corollary 12.* To obtain the expansions for $\nu \to 8\pi$, we use the first two properties in Remark 39 and the fact that we can think of the errors as uniform in $d$ to conclude that all relevant contributions to the energy are increasing in $d$. Hence, the minimum is attained at $d = 0$ in the limit $\nu \to 8\pi$. We also note that only $I_1$ and $I_3$ contribute, and a calculation of the integrals then yields the Lee–Huang–Yang constant. □

## Appendix A. Approximations to integrals

*Proof of Lemma 25.* We make a change of variables to obtain

$$\begin{aligned}b^{3/2}\int \ln\left(1 - e^{-b\sqrt{(p^2+\delta_0/b)^2+2(p^2+\delta_0/b)}}\right) dp\\ - \int \ln(1-e^{-b(p^2+\delta_0/b)})dp - b\int (e^{b(p^2+\delta_0/b)}-1)^{-1} dp.\end{aligned} \tag{A.1}$$

Regard $\delta_0/b$ as a fixed parameter and note that the integral has a limit as $b \to 0$ by the Monotone Convergence Theorem, which is

$$b^{3/2}\int \left[\frac{1}{2}\ln\left(1+\frac{2}{p^2+\delta_0/b}\right) - \frac{1}{p^2+\delta_0/b}\right] dp \le Cb^{3/2}.$$

Of course $\delta_0/b$ is not fixed, but the error term in this convergence is uniform in $\delta_0/b$ as long as that quantity is bounded (smaller than 1, say). For

$\delta_0/b \geq 1$, we expand the logarithm in the first line of (A.1) as a Taylor series around $b = 0$. Using the Mean Value Theorem and noting that the absolute value of the second derivative attains its maximum at 0, we conclude that the quantity of interest is bounded by

$$b^2 \int \frac{(p^2+\delta_0+1)e^{p^2+\delta_0}-1}{(p^2+\delta_0)(e^{p^2+\delta_0}-1)^2}dp \leq C\delta_0^{-1/2}b^2 \leq Cb^{3/2}.$$

□

*Proof of Lemma 26.* Recall $|\widehat{Vw}(p)| \leq \widehat{Vw}(0) = 8\pi a$, so that the integral converges pointwise to the desired expression as $\phi \to 0$. We would like to apply the Dominated Convergence Theorem, which leads us to analyse

$$f(t) := \frac{x+tA}{\sqrt{(x+tA)^2 - t^2A^2}} - 1,$$

where $x = p^2+d$, $A = (1+\theta)\sigma$ and $t \in [-1,1]$. This function has the property that $|f(t)| \leq f(1)$ for $t \in [0,1]$, and $|f(t)| \leq f(-1)$ for $t \in [-1,1]$ as long as $x > 2A$. We therefore dominate the function by replacing $\widehat{Vw}(\phi p)/8\pi a$ by 1 for $|p| \leq \sqrt{3(1+\theta)\sigma}$, and by $-1$ elsewhere. This function is integrable, and so the Dominated Convergence Theorem gives the desired result. To obtain uniformity, we use continuity in the different parameters. □

*Proof of Lemma 27. Step 1: first line in statement.*
We will write $s = \phi/\sqrt{T} \ll 1$. After a change of variables, we need to show that

$$\begin{aligned} T^{3/2} \int &\left( e^{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 \frac{\widehat{Vw}(\sqrt{T}p)}{8\pi a}}} - 1\right)^{-1} \\ &\times \frac{p^2+ds^2+(1+\theta)\sigma s^2 \frac{\widehat{Vw}(\sqrt{T}p)}{8\pi a}}{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 \frac{\widehat{Vw}(\sqrt{T}p)}{8\pi a}}}dp \\ = T^{3/2} \int &\left( e^{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2}} - 1\right)^{-1} \\ &\times \frac{p^2+ds^2+(1+\theta)\sigma s^2}{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2}}dp + o(T^{5/2}a^2(\rho^{1/3}a)^{-3/8}). \end{aligned}$$

We define

$$\begin{aligned} f(p,t) = &\left( e^{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t}} - 1\right)^{-1} \\ &\qquad \times \frac{p^2+ds^2+(1+\theta)\sigma s^2 t}{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t}}, \end{aligned}$$

and calculate its derivative in $t$:

$$\begin{aligned}
&\partial_t f(p,t) = \\
&= -\frac{1}{4}\sinh^{-2}\left(\frac{1}{2}\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t}\right) \\
&\qquad\qquad \times \frac{(1+\theta)\sigma s^2\left(p^2+ds^2+(1+\theta)\sigma s^2 t\right)}{p^2+ds^2+2(1+\theta)\sigma s^2 t} \\
&\quad + \left(e^{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t}}-1\right)^{-1} \\
&\qquad\qquad \times \frac{(p^2+ds^2)(1+\theta)^2\sigma^2 s^4 t}{\left((p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t\right)^{3/2}} \\
&=: F_1(p,t)+F_2(p,t).
\end{aligned}$$

We use the Mean Value Theorem to estimate

$$\begin{aligned}
&|f(p,\widehat{Vw}(\sqrt{T}p)/8\pi a)-f(p,1)| \\
&\qquad \le \left(\sup_{t\in[\widehat{Vw}(\sqrt{T}p)/8\pi a),1]}|\partial_t f(p,t)|\right)\left|\widehat{Vw}(\sqrt{T}p)/8\pi a-1\right|.
\end{aligned} \tag{A.2}$$

Before we estimate this, we make the following two observations:

(1) For $|p|\le(\rho^{1/3}a)^{-1/8}$ we have

$$|\widehat{Vw}(\sqrt{T}p)/8\pi a-1|\le C\|\widehat{Vw}''\|_\infty Tp^2\le CTa^2(\rho^{1/3}a)^{-1/4}.$$

This also means that $t(p)=\widehat{Vw}(\sqrt{T}p)/8\pi a\ge 1/2$ in this region.

(2) For $|p|\ge(\rho^{1/3}a)^{-1/8}$, we first note that in general

$$|\widehat{Vw}(\sqrt{T}p)/8\pi a)-1|\le 2.$$

We also have $|p|\ge(\rho^{1/3}a)^{-1/8}\gg 1\gg 2\sqrt{\sigma}s$, so that

$$\begin{aligned}
(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t &\ge \frac{1}{2}(p^2+ds^2)^2+p^2\left(\frac{1}{2}p^2-2(1+\theta)\sigma s^2\right) \\
&\quad + ds^2\left(p^2-2(1+\theta)\sigma s^2\right) \\
&\ge \frac{1}{2}(p^2+ds^2)^2\ge\frac{1}{2}p^4.
\end{aligned}$$

Using these estimates, and the fact that $\sinh(x)^{-1}\le 2(e^x-1)^{-1}$ for $x>0$, we estimate the contribution of $F_1$ to (A.2) by

$$\begin{cases} CTa^2(\rho^{1/3}a)^{-1/4}\left(\frac{1}{e^{|p|\sqrt{(1+\theta)\sigma s^2/2}}-1}\right)^2(1+\theta)\sigma s^2 & \text{if } |p|\le(\rho^{1/3}a)^{-1/8} \\ C\frac{1}{e^{p^2/(2\sqrt{2})}-1} & \text{if } |p|\ge(\rho^{1/3}a)^{-1/8} \end{cases},$$

and the contribution from $F_2$ by

$$\begin{cases} CTa^2(\rho^{1/3}a)^{-1/4}\frac{1}{e^{|p|\sqrt{(1+\theta)\sigma s^2}}-1} \quad \frac{1}{|p|}\sqrt{(1+\theta)\sigma s^2} \\ \qquad\qquad\qquad\qquad \text{if } |p|\le(\rho^{1/3}a)^{-1/8} \\ C\frac{1}{e^{p^2/\sqrt{2}}-1} \\ \qquad\qquad\qquad\qquad \text{if } |p|\ge(\rho^{1/3}a)^{-1/8} \end{cases}.$$

Integrating (A.2) amounts to integrating the above contributions, which gives the desired result (this can be seen after a change of variables by noting that the outer integrals decay exponentially fast), and the error is independent of $d$.

*Step 2: second line in statement.* We again write $s = \phi/\sqrt{T}$ to obtain

$$T^{3/2} I_4(d,\sigma,\theta,s) - \rho_{\mathrm{fc}} = (2\pi)^{-3} T^{3/2} s^3 \Big[ \int \left( e^{s^2\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma}} - 1 \right)^{-1} \times \frac{p^2+d+(1+\theta)\sigma}{\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma}} - \left( e^{s^2p^2} - 1 \right)^{-1} \Big] dp. \tag{A.3}$$

If we can show that this equals

$$(2\pi)^{-3} T^{3/2} s \int \Big[ \frac{p^2+d+(1+\theta)\sigma}{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma} - \frac{1}{p^2} \Big] dp + o\left(T^{3/2}s\right), \tag{A.4}$$

we would obtain the desired result by calculating the integral.

We therefore consider the difference of these two terms, and consider the regions $|p| \le B$ and $|p| > B$ separately, where $B \gg 1$ is chosen in such a way that the integrals over $|p| > B$ of (A.3) and (A.4) are $o(T^{3/2}s)$. Since the latter is a convergent integral, it is clear that this can be done. We will show the same for (A.3) in a moment.

For $|p| \le B$, we first apply the Monotone Convergence Theorem to the two terms in (A.3) separately. This shows convergence to the corresponding part of the integral (A.4).

Employing another change of variables, and writing $b = 2(d + (1+\theta)\sigma)$ and $c = d(d + 2(1+\theta))$, it remains to show that we can pick $B$ such that

$$\int_{|p|>Bs} \left| \Big[ (e^{p^2\sqrt{1+bs^2/p^2+cs^4/p^4}} - 1)^{-1} \times \frac{1+bs^2/2}{\sqrt{1+bs^2/p^2+cs^4/p^4}} - (e^{p^2}-1)^{-1} \Big] \right| dp = o(s).$$

To show this, we apply Taylor's theorem to $bs^2/p^2 + cs^4/p^4 \ll 1$, so that the above expression is bounded by

$$\frac{bs^2}{2} \int\limits_{|p|>Bs} \frac{1}{e^{p^2}-1} dp + C \int\limits_{|p|>Bs} \frac{e^{\sqrt{2}p^2}(\sqrt{2}p^2+1)-1}{(e^{p^2}-1)^2} \left( b\frac{s^2}{p^2} + c\frac{s^4}{p^4} \right) \left( 1 + b\frac{s^2}{2} \right) dp,$$

where the first term comes from the zeroth-order term, and the other from the derivative. Seeing that the main contribution from these integrals comes from $p = 0$, we conclude that this is bounded by $C(b/B + c/B^3)s$, which indicates that we can indeed pick $B$ large enough to obtain $o(s)$. □

*Proof of Lemma 28.* We would like to apply the Dominated Convergence Theorem to the limit $\phi^2 = \rho_0 a \to 0$. We have shown how to bound the fraction in Lemma 26 above. The exponential can be bounded in a similar way (i.e. by considering $|p| \le \sqrt{3(1+\theta)\sigma}$ and $|p| > \sqrt{3(1+\theta)\sigma}$ separately) since $\phi^2/T = \rho_0 a/T \ge O(1)$ by our assumptions. Uniformity follows by continuity in the different parameters. Another change of variables gives the result stated in the lemma. We obtain uniformity of the error in $d \geq 0$ since both sides of the statement are exponentially decaying in $d \gg 1$. □

*Proof of Lemma 29.* As in the proof of Lemma 26, we regard $t = \widehat{Vw}(\phi p)/8\pi a$ as a parameter taking values in $[-1, 1]$, and replace it by 1 for $|p| \leq \sqrt{3(1+\theta)\sigma}$. For other $p$, the function is continuous in $t \in [-1, 1]$, and we can maximize it for every $p$. This way, we again obtain a dominating function which is still integrable, so that we can apply the Dominated Convergence Theorem. □

*Proof of Lemma 30. Step 1: first line in statement.*
We will write $s = \phi/\sqrt{T} \ll 1$. After a change of variables, our goal is to show that

$$T^{5/2} \int \ln\left(1 - e^{-\sqrt{(p^2+ds^2)^2 + 2(p^2+ds^2)(1+\theta)\sigma s^2 \frac{\widehat{Vw}(\sqrt{T}p)}{8\pi a}}}\right) dp$$
$$= T^{5/2} \int \ln\left(1 - e^{-\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2}}\right) dp$$
$$+ O\left(T^{5/2}\phi^2 a^2 (\rho^{1/3}a)^{-1/4}\right).$$

To this end, we define

$$f(p,t) = \ln\left(1 - e^{-\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t}}\right).$$

This function is continuously differentiable in $t$:

$$\partial_t f(p,t) = \left(e^{\sqrt{(p^2+ds^2)^2+2(p^2+ds^2)(1+\theta)\sigma s^2 t}} - 1\right)^{-1}$$
$$\times \frac{(p^2+ds^2)(1+\theta)\sigma s^2}{\sqrt{(p^2+ds^2)^2 + 2(p^2+ds^2)(1+\theta)\sigma s^2 t}}.$$

We use the Mean Value Theorem to estimate this, followed by the two estimates discussed below (A.2):

$$|f(p, \widehat{Vw}(\sqrt{T}p)/8\pi a) - f(p,1)|$$
$$\leq \left(\sup_{t\in[\widehat{Vw}(\sqrt{T}p)/8\pi a, 1]} |\partial_t f(p,s,t)|\right) \left|\widehat{Vw}(\sqrt{T}p)/8\pi a - 1\right|$$
$$\leq \begin{cases} CTa^2(\rho^{1/3}a)^{-1/4}\frac{1}{e^{p^2}-1}(1+\theta)\sigma s^2 & \text{if } |p| \leq (\rho^{1/3}a)^{-1/8} \\ C\frac{1}{e^{p^2/\sqrt{2}}-1} & \text{if } |p| \geq (\rho^{1/3}a)^{-1/8} \end{cases}.$$

Integrating over $p$ gives the desired result (note that the outer integral decays exponentially fast), and the error is independent of $d$.

*Step 2: second line in statement.*
We again write $s = \phi/\sqrt{T}$ to obtain

$$T^{5/2}I_2(d,\sigma,\theta,s) - T^{5/2}f_{\min} - s^2 T\rho_{\mathrm{fc}}(d + (1+\theta)\sigma)$$
$$= (2\pi)^{-3}T^{5/2}s^3 \int \left[\ln\left(1 - e^{-s^2\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma}}\right)\right. \tag{A.5}$$
$$\left. - \ln\left(1 - e^{-s^2p^2}\right) - (e^{s^2p^2} - 1)^{-1}(d + (1+\theta)\sigma)s^2\right] dp.$$

Since this expression divided by $T^{5/2}s^3$ is monotone in $s$, we obtain by the Monotone Convergence Theorem that

$$(2\pi)^{-3}T^{5/2}s^3 \int \Big[ \ln\left( \frac{\sqrt{(p^2+d)^2 + 2(p^2+d)(1+\theta)\sigma}}{p^2} \right) - \frac{d+(1+\theta)\sigma}{p^2} \Big] dp \\ + o(T^{5/2}s^3), \tag{A.6}$$

which gives the desired result.

□

*Proof of Lemma 31.* We want apply the Dominated Convergence Theorem to the limit $\phi^2 a = \rho_0 a^2 \to 0$. As in Lemma 26, we regard $t = \widehat{Vw}(\phi p)/8\pi a \in [-1,1]$ as a parameter, which we replace by 0 for $|p| \leq \sqrt{3(1+\theta)\sigma}$. For $|p| > \sqrt{3(1+\theta)\sigma}$, we replace it by $-1$ to obtain a dominating function (also using $s \geq O(1)$). Uniformity in the different parameters follows from continuity in these parameters. Another change of variables gives the desired result. We obtain uniformity of the error in $d \geq 0$ since both sides of the statement are exponentially decaying in $d \gg 1$. □

*Proof of Lemma 32.* The basic estimates we will use are:

$$\begin{aligned}
&\left| \rho_0 \int\limits_{|p|\leq b} \gamma(p)\widehat{V}(p)dp - \widehat{V}(0)\rho_0 \int\limits_{|p|\leq b} \gamma(p)dp \right| \leq Ca^3 b^2 \rho_0 \rho_\gamma \\
&\left| \rho_0 \int\limits_{|p|> b} \gamma(p)\widehat{V}(p)dp - \widehat{V}(0)\rho_0 \int\limits_{|p|> b} \gamma(p)dp \right| \leq Ca\rho_0 \int_{p>b} \gamma(p)dp \\
&\left| \iint\limits_{|p|,|q|\leq b} \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \widehat{V}(0) \left( \int\limits_{|p|\leq b} \gamma(p)dp \right)^2 \right| \leq Ca^3 b^2 \rho_\gamma^2 \\
&\left| \iint\limits_{|p|\mathrm{or}|q|> b} \gamma(p)\widehat{V}(p-q)\gamma(q)dpdq - \iint\limits_{|p|\mathrm{or}|q|> b} \gamma(p)\widehat{V}(0)\gamma(q)dpdq \right| \\
&\qquad\qquad\qquad\qquad \leq Ca\rho_\gamma \int_{|p|>b} \gamma(p)dp,
\end{aligned} \tag{A.7}$$

which follow from the fact that $\|\widehat{V}\|_\infty \leq 8\pi a$, $\widehat{V}'(0) = 0$ and $\|\widehat{V}''\|_\infty \leq Ca^3$. We also need identical versions of the first two estimates for $\widehat{Vw}$, which hold for the same reasons.

We set $b = \sqrt{T}$. By Lemma 26, we have

$$\int_{|p|>\sqrt{T}} \gamma^{\rho_0,\delta}(p)dp = O(\phi^3), \tag{A.8}$$

since the density becomes (5.18) after a change of variables and both terms are of this order (the exponent of the exponential in the second contribution is at least of order 1). This suffices to prove the statement. □

*Proof of Lemma 33.* Using the estimates in the previous proof, the reader can check that $b = \rho^{1/3}$ suffices, since

$$\int_{|p|>\rho^{1/3}} \gamma^{\rho_0,\delta} = o((\rho_0 a)^{3/2}).$$

This follows from an application of the Dominated Convergence Theorem to

$$(\rho_0 a)^{3/2} \int_{|p|>\frac{\rho^{1/3}}{\sqrt{\rho_0 a}}} \left( \frac{p^2 + d + \frac{\widehat{Vw}(\sqrt{\rho_0 a}p)}{a}}{\sqrt{(p^2+d)^2 + 2(p^2+d)\frac{\widehat{Vw}(\sqrt{\rho_0 a}p)}{a}}} - 1 \right) dp$$

as in Lemma 26, and the fact that the other contribution in (5.18) is exponentially small in this region (since $\rho^{1/3} \gg \sqrt{T}$). □

*Proof of Lemma 34. Step 1.* We start by looking at the first term in (5.52), which does not involve $\phi^2/T$. After adding absolute values within the integral sign, we employ similar reasoning to Lemma 26 to conclude that it is $O(\phi^3)$ as $\phi \to 0$. Similar to (A.8), we then have

$$\int\limits_{|p|>\sqrt{T}} |f(p)| dp \leq C\phi^3,$$

which was one of our goals.

*Step 2.* We now restrict to the case $\phi^2/T \ll 1$ and consider the full integral of $f$. Again using that the first term in (5.52) only contributes $O(\phi^3)$, we have that

$$\begin{aligned} \int f(p) dp = \phi^3 \int & \frac{(1+\theta)\sigma \frac{\widehat{Vw}(\phi p)}{8\pi a}}{\sqrt{(p^2+d)^2 + 2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}} \\ & \times \frac{1}{e^{\frac{\phi^2}{T}\sqrt{(p^2+d)^2+2(p^2+d)(1+\theta)\sigma\frac{\widehat{Vw}(\phi p)}{8\pi a}}} - 1} dp \\ & + O(\phi^3) \\ = T\phi \int & \frac{(1+\theta)\sigma}{(p^2+d)^2 + 2(p^2+d)(1+\theta)\sigma} dp + o(T\phi) \\ = T\phi & (1+\theta)\sigma \frac{2\pi^2}{\sqrt{d+2(1+\theta)\sigma} + \sqrt{d}} + o(T\phi). \end{aligned} \tag{A.9}$$

The step before the last requires reasoning similar to Lemma 29, where the application of the Dominated Convergence Theorem is facilitated by the fact that $(e^x - 1)^{-1} \leq x^{-1}$.

An identical argument leads to the estimate that $\int |f| \leq CT\phi$.

*Step 3.* For the case $\phi^2/T \geq O(1)$, the second line in (A.9) combined with the Dominated Convergence Theorem applied as in Lemma 28 leads to the desired conclusion. □

*Proof of Lemma 35.* We first analyse the asymptotic behaviour of $F^{(1)}$ as $d \to \infty$. Writing $A(p) = \widehat{Vw}(\phi p)/a$, we expand for $d \gg A = O(1)$:

$$(p^2+d)\sqrt{1+\frac{2A}{p^2+d}} = p^2+d+A-\frac{1}{2}\frac{A^2}{p^2+d}+o(A/d).$$

This tells us that the asymptotic behaviour of $F^{(1)}$ is

$$(2\pi)^{-3}d\phi^5\frac{1}{4}\int A^2(p)\frac{1}{p^2(p^2+d)}dp.$$

Similarly, we can see that the asymptotic behaviour of $-d\phi^2\rho_\gamma^{(1)}$ is

$$-(2\pi)^{-3}d\phi^5\frac{1}{4}\int A^2(p)\frac{1}{(p^2+d)^2}dp. \tag{A.10}$$

By our assumptions on the derivative of the potential, there exists a $c$ such that $|\widehat{Vw}(p)| \geq 4\pi a$ for $|p| \leq c/a$. Hence, for $d^{1/2}\phi a \leq C$, the two sum of the two contributions above is bounded below by

$$Cd^{1/2}\phi^5 \int\limits_{|p|\leq c(d^{1/2}\phi a)^{-1}} \frac{\widehat{Vw}^2(d^{1/2}\phi p)a^{-2}}{p^2(p^2+1)^2}dp \geq Cd^{1/2}\phi^5,$$

whereas for $d^{1/2}\phi a \geq C$, it is bounded below by

$$d^2\phi^5(\phi a)^3\int_{|p|\leq c}\frac{\widehat{Vw}^2(p/a)a^{-2}}{p^2(p^2+d\phi^2a^2)^2}dp \geq Ca^{-1}\phi^4.$$

To prove the claims about $\rho_\gamma^{(1)}$ we first consider $d \gg 1$ and use (A.10) (divided by $d\phi^2$). On the remaining compact $0 \leq d \leq C$, we can apply Lemma 26. □

*Proof of Lemma 37.* Let $\sqrt{T} \ll b \ll \sqrt{T}(\sqrt{T}a)^{-1/8}$. Using (A.8), we first notice that

$$\iint_{|p|\text{or}|q|>b}\gamma^{\rho_0,\delta}(p)\widehat{V}(p-q)\gamma^{\rho_0,\delta}(q)dpdq \leq Ca\rho\phi^3 = o(T^4a^3).$$

The same holds for the similar contribution to $E_5$ involving $\widehat{V}(0)$. Using (5.44) and (5.19), we see that the final contribution to the outer region is also $o(T^4a^3)$ since

$$\int_{|p|>b}\gamma_0 = o(T^{3/2}), \qquad \int_{|p|>b}p^2\gamma_0 = o(T^{5/2}).$$

We again use (5.44) and estimate the contribution from the inner region by

$$C\Big|\iint\limits_{|p|,|q|\leq b}\gamma^{\rho_0,\delta}(p)\left(\widehat{V}(p-q)-\widehat{V}(0)-\frac{\Delta\widehat{V}(0)|p-q|^2}{6}\right)\gamma^{\rho_0,\delta}(q)dpdq\Big|$$
$$+C\Delta\widehat{V}(0)\rho_{\gamma^{\rho_0,\delta}}\int\limits_{|p|\leq b}p^2|\gamma^{\rho_0,\delta}-\gamma_0|(p)dp$$
$$+C\Delta\widehat{V}(0)\left(\int\limits_{|p|\leq b}|\gamma^{\rho_0,\delta}-\gamma_0|(p)dp\right)\left(\int\limits_{|p|\leq b}p^2\gamma_0(p)dp\right).$$

Lemmas 26 and 27 (where also the proof of Lemma 27 is important to deal with the absolute value for the middle term) together with the properties of $\gamma_0$ and the properties of the potential pointed out below (A.7) imply that this is indeed $o(T^4a^3)$. □

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