The free energy of a dilute two-dimensional Bose gas

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Abstract

We study the interacting homogeneous Bose gas in two spatial dimensions in the thermodynamic limit at fixed density. We shall be concerned with some mathematical aspects of this complicated problem in many-body quantum mechanics. More specifically, we consider the dilute limit where the scattering length of the interaction potential, which is a measure for the effective range of the potential, is small compared to the average distance between the particles. We are interested in a setting with positive (i.e., non-zero) temperature.

After giving a survey of the relevant literature in the field, we provide some facts and examples to set expectations for the two-dimensional system. The crucial difference to the three-dimensional system is that there is no Bose–Einstein condensate at positive temperature due to the Hohenberg–Mermin–Wagner theorem. However, it turns out that an asymptotic formula for the free energy holds similarly to the three-dimensional case. We motivate this formula by considering a toy model with δ interaction potential. By restricting this model Hamiltonian to certain trial states with a quasi-condensate we obtain an upper bound for the free energy that still has the quasi-condensate fraction as a free parameter. When minimizing over the quasi-condensate fraction, we obtain the Berezinskii–Kosterlitz–Thouless critical temperature for superfluidity, which plays an important role in our rigorous contribution.

The mathematically rigorous result that we prove concerns the specific free energy in the dilute limit. We give upper and lower bounds on the free energy in terms of the free energy of the non-interacting system and a correction term coming from the interaction. Both bounds match and thus we obtain the leading term of an asymptotic approximation in the dilute limit, provided the thermal wavelength of the particles is of the same order (or larger) than the average distance between the particles. The remarkable feature of this result is its generality: the correction term depends on the interaction potential only through its scattering length and it holds for all nonnegative interaction potentials with finite scattering length that are measurable. In particular, this allows to model an interaction of hard disks.

About the author

Simon Mayer received a Bachelor of Science in Physics from the Eberhard Karls University of Tübingen, Germany, in 2013. In his Bachelor thesis, titled “About a two-body interaction of fermions”, he investigated a problem in many-body quantum mechanics.

He went on to study at the University of Cambridge, United Kingdom, and obtained a Master of Advanced Studies in Applied Mathematics in 2014. At the University of Cambridge, Simon attended lectures in theoretical physics as well as pure and applied mathematics. He joined the graduate school of IST Austria in the fall of 2014.

During his PhD, Simon furthered his studies on mathematical aspects of many-body quantum mechanics and in particular dilute Bose gases.

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List of publications

This thesis contains the following publications:

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2. S. Mayer and R. Seiringer. "The free energy of the two-dimensional dilute Bose gas. II. Upper bound" (2020), in preparation.

Contents

1 Introduction to dilute Bose gases

In this chapter we give an overview of the mathematical literature on dilute Bose gases and present the statement of the main theorem concerning an asymptotic expansion of the free energy of a two-dimensional Bose gas in the dilute limit. To motivate the formula appearing in the theorem, we consider a toy model with δ interaction. Restricting this model Hamiltonian to a certain class of trial states that have a coherent state in the $p = 0$ mode, we obtain an upper bound on its free energy. When minimizing this upper bound over the condensate fraction, the Berezinskii–Kosterlitz–Thouless critical temperature for superfluidity appears as the important temperature scale. We further highlight the differences between the two- and three-dimensional system and sketch the strategy that will be used in Chapter 2 and 3 to give the proof of the main theorem.

1.1 A survey of the literature

Einstein [24] reported already in 1924 and 1925 about the possibility of condensation of a system of particles obeying Bose statistics into the ground state. His work was based on Bose's derivation [12] of Planck's radiation law, and was long thought to be of academic interest only. In fact, it took seventy years until Bose–Einstein condensation (BEC) could be experimentally observed in dilute alkali gases [3, 18], which are however interacting systems. Einstein's original result was valid for an ideal Bose gas only and it is a famous open problem in mathematical physics to show BEC for general interacting systems. There is a vast body of works on BEC: see the reviews [15, 17, 33, 40, 80] and monographs [62, 63], for example. For an overview of some recent rigorous results, see [46], for a shorter introduction see [72].

The first rigorous advances were made for proving the ground state energy of a dilute three-dimensional Bose gas in the thermodynamic limit at fixed density. The leading order of the ground state energy per unit volume is given by

$$e^{3\mathrm{D}}(\rho) = 4\pi a\rho^2(1 + o(1)), \tag{1.1.1}$$

where ρ is the average density of the gas and a denotes the scattering length of the interaction potential. This formula becomes exact in the dilute limit $a^3\rho \to 0$, where the scattering length is small compared to the average interparticle distance. Dyson [23] proved an upper bound for hard spheres but his lower bound was still off by a factor. The correct lower bound was proved much later by Lieb and Yngvason [51], which now can be considered a major mathematical breakthrough. An upper bound for general interaction potentials was given in [47]. Remarkably, the ground state energy depends to leading order only on the interaction potential through the scattering length.

The second order correction to the ground state energy in the dilute limit was also found to depend only on the scattering length. Up to the order $(a^3\rho)^{1/2}$, the formula for the ground state energy reads

$$e^{3\mathrm{D}}(\rho) = 4\pi a\rho^2\left(1 + \frac{128}{15\sqrt{\pi}}(a^3\rho)^{1/2} + o((a^3\rho)^{1/2})\right). \tag{1.1.2}$$

The form of the correction term was initially predicted by Lee, Huang and Yang [39] and much effort has been put forward through the years to prove it rigorously. To mention only a few, Lieb [42] obtained the LHY correction but used additional (non-rigorous) assumptions, [25] still has a multiplicative factor in an upper bound on the correction term and [29] shows the LHY correction in a high density regime. See [10] for related work on the Gross–Pitaevskii limit. The first rigorous upper bound for the LHY correction was proved by Yau and Yin [78] for smooth interaction potentials with fast decay, while the lower bound was proved only recently by Fournais and Solovej in [28], building on the work of [13, 14]. Since the authors of [28] assume the interaction potential to be of L^1-type with compact support (which is the most general proof yet), the LHY correction is still to be proved for a hard sphere interaction. For predictions of even higher order corrections to these formulas, we refer the reader to [43, 53, 77].

In the influential paper [11], Bogoliubov introduced his approximation scheme, which yields the integral of the potential for the ground state energy in the dilute regime. It was only due to Landau (whom Bogoliubov thanks in a footnote) that to obtain the correct result one has to manually replace the integral of the potential by the scattering length. For a modern review of the Bogoliubov theory, see [81]. There have been many works on the validity of Bogoliubov's approximation in a many-body setting: See, for example, the articles [49, 50, 75], which studied the one- and two-component charged Bose gas. In the case of an external trapping potential, even the excitation spectrum was analyzed, see [19, 30, 41, 56, 71]. More recently, in a confined setting in combination with the Gross–Pitaevskii limit, the ground state energy as well as the excitation spectrum could be obtained [8–10].

At positive temperature, the analogous quantity to the ground state energy is the free energy. In the thermodynamic limit the leading order contribution to the free energy in three dimensions coming from the interaction has been found to be

$$f^{3\mathrm{D}}(\beta,\rho) = f_0^{3\mathrm{D}}(\beta,\rho) + 4\pi a\rho^2\left(2 - \left[1 - \left(\frac{\beta_{\mathrm{c}}^{3\mathrm{D}}(\rho)}{\beta}\right)^{3/2}\right]_+^2\right)(1 + o(1)). \tag{1.1.3}$$

Here, $f_0^{3\mathrm{D}}(\beta,\rho)$ is the free energy of non-interacting bosons in three dimensions, $[\,\cdot\,]_+ = \max\{0,\cdot\}$ denotes the positive part, $\beta = 1/T$ is the inverse temperature and $\beta_{\mathrm{c}}^{3\mathrm{D}} = \zeta(3/2)^{2/3}/(4\pi\rho^{2/3})$ is the inverse critical temperature for BEC of the ideal Bose gas in three dimensions. The form of the interaction term can be understood in an intuitive way and results from the bosonic nature of the particles. Two bosons in different one-particle wavefunctions feel an exchange effect that increases their interaction energy by a factor of two compared to when they are in the same one-particle wavefunction. The $[\,\cdot\,]_+$ bracket equals the condensate fraction of the ideal gas, which is to leading order also the fraction of particles that do not feel an exchange effect.

See [79] for the proof of the upper bound and [70] for the proof of the lower bound. It is valid in case $\beta\rho^{2/3} \gtrsim 1$, i.e., if the temperature is of the order of the critical temepratures of the ideal gas or lower. There is a recent result about the free energy asymptotics in the Gross–Pitaevskii limit in a box [21], as well as in a trapped setting [22], where the limit is a combined Gross–Pitaevskii and thermodynamic limit. The positive temperature situation was further studied in [27, 57–59], where the Hamiltonian was restricted to quasi-free states. These articles contain formulas for the energy and critical temperature that are conjecturally valid in a combined dilute and weak-coupling limit.

Finally, we discuss the two-dimensional system, which is the main point of interest of this thesis. The leading order term for the ground state energy per unit volume in the dilute limit is given by

$$e^{2\mathrm{D}}(\rho) = \frac{4\pi\rho^2}{|\ln a^2\rho|}(1 + o(1)). \tag{1.1.4}$$

The error term is small in case the dimensionless parameter $a^2\rho$ is small or, in other words, if the scattering length is small compared to the average interparticle distance. It was first predicted by Schick [67], another derivation is due to Ovchinnikov [61] (using essentially Lieb's method [42]). However, it was not until 2001 that the asymptotics for the ground state energy in the thermodynamic limit was proved rigorously by Lieb and Yngvason [52]. In contrast to the three-dimensional case, the two-dimensional ground state energy is *not* the sum of the ground state energy of $N(N-1)/2$ pairs of particles and the coupling parameter $|\ln a^2\rho|^{-1}$ depends explicitly on the density. The next order correction to (1.1.4) is predicted to be of the form

$$-4\pi\rho^2 \frac{\ln|\ln a^2\rho|}{|\ln a^2\rho|}, \tag{1.1.5}$$

see, e.g., [2, 16].

At positive temperature, the situation for the two-dimensional system has until now not been so well understood. Proving the leading order of the free energy asymptotics in the thermodynamic limit has been an open problem and it is this gap that is closed below in Chapters 2 and 3 of the present thesis. We show that the free energy per unit volume satisfies

$$f^{2\mathrm{D}}(\beta,\rho) = f_0^{2\mathrm{D}}(\beta,\rho) + \frac{4\pi\rho^2}{|\ln a^2\rho|}\left(2 - \left[1 - \frac{\beta_{\mathrm{c}}^{2\mathrm{D}}(\rho,a)}{\beta}\right]_+^2\right)(1 + o(1)), \tag{1.1.6}$$

where $f_0^{2\mathrm{D}}$ is the free energy of non-interacting bosons in two dimensions and $\beta_{\mathrm{c}}^{2\mathrm{D}}(\rho,a)$ is defined by

$$\beta_{\mathrm{c}}^{2\mathrm{D}}(\rho,a) = \frac{\ln|\ln a^2\rho|}{4\pi\rho}. \tag{1.1.7}$$

We note that (the inverse of) $\beta_{\mathrm{c}}^{2\mathrm{D}}(\rho,a)$ coincides with the Berezinskii–Kosterlitz–Thouless critical temperature for superfluidity found in the physics literature, see [6, 7, 36, 37] for the original publications. The term $\rho[1 - \beta_{\mathrm{c}}^{2\mathrm{D}}(\rho,a)/\beta]_+$ has the physical interpretation of a superfluid density [26]. For a discussion of the physics of the superfluid phase transition in the two-dimensional Bose gas we refer to [64]. It should be noted that the inverse critical temperature $\beta_c^{2D}(\rho, a)$ depends directly on the interaction potential via its scattering length as opposed to in three dimensions, where the critical temperature for BEC of the ideal gas appears in the formula for the free energy. In fact, since the Mermin–Wagner–Hohenberg theorem [32, 55] excludes Bose–Einstein condensation at positive temperatures, we cannot expect a similar behavior in our case. There is a rigorous upper bound [73] on the critical temperature of a dilute two-dimensional Bose gas which coincides with the critical temperature for superfluidity to leading order. The definition of criticality in that article is the condition that the decay of correlations changes from exponential decay above the critical temperature to power law decay below it. To the best of our knowledge, the formula for the free energy asymptotics of the two-dimensional system (1.1.6) does not seem to have appeared explicitly in the literature before. It should be possible to obtain it from the analysis in [26], however.

We give explicit bounds on the $o(1)$ correction in (1.1.6) below in case $a^2\rho \ll 1$ and $\beta\rho$ of order one or larger, see the statement of Theorem 1. In other words, the free energy is given to leading order as above when the scattering length is small compared to the average interparticle distance and the thermal wavelength of the particles is larger than or equal to the average interparticle distance. See [20] and [54] for the original works this thesis is based on.

As a side remark we mention that there are also several works on interacting fermionic systems. The ground state energy in the dilute limit has been analyzed in [45] and the free energy at positive temperature was studied in [69] (actually the main result in [69] is stated for the pressure but in a corollary it is shown that this implies the asymptotics for the free energy as well). While [45] studied also the two-dimensional system, in [69] only the three-dimensional system was considered. Proving the free energy correction for a dilute two-dimensional Fermi gas is still an open problem.

1.2 Presentation of the main theorem

In this section, we present the main result of this thesis, Theorem 1. In the following we will deal only with the two-dimensional system and therefore we drop the superscript "2D" on the two-dimensional free energies f^{2D}, f_0^{2D} and the critical temperature β_c^{2D}. In order to precisely state the result, we first discuss the necessary preliminaries. We specify the model that we use, define the specific free energy in the thermodynamic limit (for the interacting system as well as the free gas) and define the scattering length.

We consider the Hamiltonian for N bosons in a two-dimensional torus Λ, given by

$$H_N = -\sum_{i=1}^{N} \Delta_i + \sum_{i<j}^{N} v(d(x_i, x_j)), \tag{1.2.1}$$

where Δ_i is the Laplacian on Λ for the i-th particle, $d(x, y)$ is the distance function on the torus and $v \geq 0$ is a nonnegative two-body interaction potential with finite scattering length a (to be defined properly below), which we assume to be measurable. The interaction potential is allowed to take the value $+\infty$ (on a set of nonzero measure), which in particular permits to model an interaction of hard disks. This Hamiltonian acts on the symmetric tensor product of square integrable functions on the torus

$$\mathcal{H}_N = \bigotimes_{\text{sym}}^{N} L^2(\Lambda). \tag{1.2.2}$$

We will describe the torus Λ as a square of side length L embedded in the plane with opposing sides identified, i.e., we have $\Lambda = [0, L]^2 \subset \mathbb{R}^2$. Then Δ is the usual Laplacian on $[0, L]^2$ with periodic boundary conditions and the distance function $d(x, y)$ is explicitly given as

$$d(x, y) = \min_{k \in \mathbb{Z}^2} |x - y - kL|. \tag{1.2.3}$$

The quantity of interest is the free energy per unit volume of the system as a function of the inverse temperature $\beta = 1/T$ and density ρ defined by

$$f(\beta, \rho) = -\frac{1}{\beta} \lim_{\substack{N,L\to\infty \\ N/L^2=\rho}} \frac{1}{L^2} \ln \operatorname{Tr}_{\mathcal{H}_N} \mathrm{e}^{-\beta H_N}. \tag{1.2.4}$$

The limit is the usual thermodynamic limit[1] of large particle number and large volume while keeping the density fixed. The free energy asymptotics we will give applies to the setting of a dilute gas, where the parameter $a^2\rho$ is small while $\beta\rho$ is of order one or larger. In other words, the scattering length is supposed to be small compared to the average particle distance while the thermal wave length of the particles is of the same order as the average particle distance or larger.

For non-interacting bosons, the free energy can be calculated explicitly. One has to solve the maximization problem

$$f_0(\beta, \rho) = \sup_{\mu \leq 0} \left\{ \mu\rho + \frac{1}{4\pi^2\beta} \int_{\mathbb{R}^2} \ln\left(1 - \mathrm{e}^{-\beta(p^2-\mu)}\right) \mathrm{d}p \right\}. \tag{1.2.5}$$

[1] Existence of this limit (and independence of the boundary conditions used) can be shown by standard techniques, see, e.g., [65, 66].

The chemical potential μ_0 that maximizes the free energy satisfies the equation

$$\frac{1}{4\pi^2}\int_{\mathbb{R}^2}\frac{\mathrm{d}p}{\mathrm{e}^{\beta(p^2-\mu_0)}-1}=\rho \tag{1.2.6}$$

and therefore

$$\mu_0(\beta,\rho)=\frac{1}{\beta}\ln\left(1-\mathrm{e}^{-4\pi\beta\rho}\right). \tag{1.2.7}$$

This corresponds to the following explicit form of the free energy

$$f_0(\beta,\rho)=\rho^2\left[\frac{1}{\beta\rho}\ln\left(1-\mathrm{e}^{-4\pi\beta\rho}\right)-\frac{1}{4\pi(\beta\rho)^2}\,\mathrm{Li}_2\left(1-\mathrm{e}^{-4\pi\beta\rho}\right)\right], \tag{1.2.8}$$

where

$$\mathrm{Li}_2(z)=-\int_0^z\frac{\ln(1-t)}{t}\,\mathrm{d}t \tag{1.2.9}$$

is the polylogarithm of order 2 (also called the dilogarithm). From this expression for the free energy of free bosons we directly obtain the scaling relation

$$f_0(\beta,\rho)=\rho^2 f_0(\beta\rho,1). \tag{1.2.10}$$

In particular, we see that for the free system the dimensionless parameter $\beta\rho$ completely determines (up to a factor of ρ^2) the free energy. We have the asymptotic behavior

$$\begin{aligned} f_0(x,1)&=-\frac{\pi}{24x^2}\left(1+O(\mathrm{e}^{-4\pi x})\right) &&\text{as } x\to\infty,\\ f_0(x,1)&=-\frac{1}{x}\left(1-\ln(4\pi x)\right)-\pi+O(x) &&\text{as } x\to 0. \end{aligned} \tag{1.2.11}$$

The scattering length a is defined by a variational principle, see [52, Appendix A]. We will assume here that the potential is non-negative and has a finite range R_0, i.e., we have $v(r)=0$ for $r>R_0$. Then for $R>R_0$, we define the scattering length of v by

$$\frac{2\pi}{\ln(R/a)}=\inf_g\left\{\int_{B_R}|\nabla g|^2+\frac{v}{2}|g|^2\right\}, \tag{1.2.12}$$

where the infimum is taken over functions $g\in H^1(B_R)$ with value one on the boundary, i.e., they satisfy $g|_{|x|=R}=1$. Here, $B_R\subset\mathbb{R}^2$ denotes the disk of radius R centered at the origin. The unique function g_0 that attains the infimum on the right-hand side of (1.2.12) is nonnegative, radially symmetric and satisfies the equation

$$-2\Delta g_0+vg_0=0 \tag{1.2.13}$$

in the sense of distributions on B_R. Outside the range of the potential, i.e., for $R_0 < r < R$, the minimizer g_0 is explicitly given by

$$g_0(r) = \frac{\ln(r/a)}{\ln(R/a)}. \tag{1.2.14}$$

As noted in the remark after the proof of [52, Lemma A.1], the definition of the scattering length can be extended to potentials of infinite range by cutting off the potential at a finite range and then letting the cutoff grow to infinity. From [38, Lemma 1], we know that finiteness of the scattering length is equivalent to a certain integrability condition of the potential. More precisely, if $a < \infty$, then

$$\int_{|x|>a} v(|x|) \ln^2(|x|/a)\, \mathrm{d}x < \infty \tag{1.2.15}$$

holds. Conversely, if (1.2.15) holds with a replaced by some $b > 0$, then the scattering length of the potential is finite.

We remark also that defining the scattering length via this variational principle makes sense for potentials that are not necessarily nonnegative. One has to assume that $-\Delta + v/2$ as an operator on $L^2(\mathbb{R}^2)$ has no negative spectrum, however.

The main result of this thesis is an asymptotic expansion of the free energy in terms of the free energy of non-interacting bosons and a correction term coming from the interaction as stated in (1.1.6). This is the two-dimensional analogue of (1.1.3), which itself can be obtained by combining [70, Theorem 1] (lower bound) and [79, Theorem 1] (upper bound). The expansion is meaningful for small $a^2\rho$ and $\beta\rho$ fixed or large. We introduce here the notation $x \lesssim y$ to indicate that there exists a constant $C > 0$, independently of x and y, such that $x \leq Cy$ (and analogously for "$\gtrsim$"). If $x \lesssim y$ and $y \lesssim x$ we write $x \sim y$.

Theorem 1 (Free energy asymptotics of dilute two-dimensional Bose gas)**.** *Assume that the interaction potential satisfies $v \geq 0$ and has a finite scattering length a. In the limit $a^2\rho \to 0$ where $\beta\rho \gtrsim 1$ is fixed or large, we have*

$$f(\beta,\rho) = f_0(\beta,\rho) + \frac{4\pi\rho^2}{|\ln a^2\rho|}\left(2 - \left[1 - \frac{\beta_{\mathrm{c}}(\rho,a)}{\beta}\right]_+^2\right)(1 + o(1)), \tag{1.2.16}$$

with

$$o(1) \sim \frac{\ln\ln|\ln a^2\rho|}{\ln|\ln a^2\rho|}. \tag{1.2.17}$$

Here, $[\,\cdot\,]_+ = \max\{\cdot\,, 0\}$ denotes the positive part and the inverse critical temperature $\beta_{\mathrm{c}}(\rho,a)$ is defined in (1.1.7).

We have the following remarks about the main theorem.

1. The lower bound is joint work with Andreas Deuchert and Robert Seiringer [20], while the upper bound is joint work with Robert Seiringer [54].

2. The statement on the $o(1)$ error term is uniform in $\beta\rho$ as long as $\beta\rho \gtrsim 1$. The proof of the lower bound will show that the actual error rate is much better for $\beta\rho$ some distance away from $\beta_c\rho$ (either above or below), see (2.18.16). For very low temperatures, we utilize the proof method of [52] and in this way recover the ground state energy error rate $|\ln a^2\rho|^{-1/5}$ for very low temperatures, which was proved for $T = 0$ in [52].

3. The statement is uniform in the interaction potential in the following sense. In case of finite range potentials the error term depends on the interaction potential only through its scattering length a and its range R_0. This dependence could be displayed explicitly. To prove the theorem for infinite range potentials with a finite scattering length one has to cut the potential at some radius R_0, which results in an error term (contained in the $o(1)$ in (1.2.16)) of the form

$$\frac{1}{|\ln a^2\rho|}\int_{|x|>R_0} v(|x|)\ln^2(|x|/a_{R_0})\,\mathrm{d}x, \tag{1.2.18}$$

   where a_{R_0} is the scattering length of the potential with cutoff. When R_0 is chosen such that $a_{R_0} \neq 0$, this term is much smaller than the main error term (1.2.17), but is non-uniform in the potential since a_{R_0} depends on v. Note that in contrast to the three-dimensional case one does not need to choose $R_0/a \gg 1$. How one obtains (1.2.18) is explained in detail in Lemma 2 below.

4. Even though the temperature dependence of the correction term in (1.2.16) looks very similar to the three-dimensional case, the situation is actually rather different here. While it is possible in three dimensions to obtain a term of the correct form by naive perturbation theory only (with $(8\pi)^{-1}\int v$ in place of the scattering length), this method fails in two dimensions. One would similarly obtain the integral of the potential as a factor in the correction term, which does *not* yield the correct behavior in the density (namely the inverse logarithmic factor $|\ln a^2\rho|$). Furthermore, the temperature dependence in the correction term would come out wrong, as the critical temperature for Bose–Einstein condensation (of the non-interacting system) is equal to zero in two dimensions, hence a factor of two (compared with at zero temperature) would appear at any $T > 0$. In other words, in two dimensions a naive perturbation

theory would yield

$$f_0(\beta,\rho) + 2\rho^2 \int v(|x|)\,\mathrm{d}x, \tag{1.2.19}$$

which is far from the truth. We note that the second term is infinite in the case of hard disks.

5. The main ingredient to obtain the temperature dependence in the interaction term in (1.2.16) is the variational principle

$$\inf_{0\le\rho_0\le\rho}\left\{f_0(\beta,\rho-\rho_0) + \frac{4\pi}{|\ln a^2\rho|}\left(2\rho^2-\rho_0^2\right)\right\} = f_0(\beta,\rho) + \frac{4\pi}{|\ln a^2\rho|}\left(2\rho^2-\rho_{\mathrm{s}}^2\right)(1-o(1)) \tag{1.2.20}$$

as $a^2\rho \to 0$. To leading order, the optimal choice of ρ_0 turns out to be $\rho_{\mathrm{s}} = \rho[1-\beta_{\mathrm{c}}(\rho,a)/\beta]_+$, which coincides with the superfluid density of the system [26]. One key ingredient of the proof of the lower bound for the free energy is a c-number substitution for low momentum modes. These modes are described by coherent states that do not experience an exchange effect, which decreases their energy relative to the energy of the high momentum modes that have not been substituted. The c-number substituted modes take the role of ρ_0 and one obtains a formula for the energy that is approximately given by the left-hand side of (1.2.20). In the proof of the upper bound the variational principle (1.2.20) emerges by construction of a suitable trial state that is inserted into the free energy functional.

6. It is possible to extend the theorem to particles with internal degrees of freedom. However, we consider here for simplicity the case of spinless bosons only.

The proof of Theorem 1 is given in two parts below, see Chapter 2 for the lower bound and Chapter 3 for the upper bound. In the remainder of this chapter, we will give a brief sketch of the strategy that will be used to prove the main theorem. Following that we show how a term on the left-hand side (inside the infimum) of (1.2.20) can be obtained by considering a toy model with delta interaction and how to minimize over ρ_0 to obtain the right-hand side in the dilute limit. We conclude by presenting calculations for the ground state energy and scattering length of the finite potential well in two dimensions (to set the stage for what can be expected in the two-dimensional system) and finally summarize the differences between the two- and three-dimensional system.

1.3 Sketch of the proof of the main theorem

In this section we give a brief sketch of the proof of the lower and upper bound, respectively. Below, in Sections 2.2 and 3.2, we will give an extended proof sketch with more details for the proof of the lower and upper bound.

The proof of the lower bound is based on the fact that the free energy of the non-interacting system $f_0(\beta,\rho)$ is much bigger than the interaction energy (which is the second term on the right-hand side of (1.2.16) and is proportional to $\rho^2/|\ln a^2\rho|$) in the dilute limit. However, as explained in Remark 4 above, one cannot apply a simple version of perturbation theory to obtain the result. The interaction potential is so strong such that a Gibbs state of the ideal gas would have an energy that is too large and furthermore simple perturbation theory does not give the desired temperature dependence of the interaction term (compare (1.2.16) with (1.2.19)). Therefore, a version of Dyson's Lemma [23] is used to replace the strong potential by a softer one with longer range. Then we apply a rigorous version of first order perturbation theory at positive temperature (which was developed in [70] and is based on a correlation inequality from [68]) after suitably adapting it to the two-dimensional system. This method requires that highly occupied low momentum modes have to be treated with a c-number substitution: Creation and annihilation operators of the low momentum modes are replaced by complex numbers using coherent states on the bosonic Fock space. These modes then lead to the correct temperature dependence of the interaction term, as described in Remark 5 above.

For the proof of the upper bound we employ a variational principle for the free energy. We use the fact that *any* admissible state leads to an upper bound and insert a particular trial state into the free energy functional. The trial state we are going to use consists of three parts: The thermal Gibbs state of the non-interacting system, a coherent state and a product function (Jastrow factor [34]) that adds a correlation structure to the system. We are then able to extract the two terms occurring on the left-hand side of (1.2.20) and by minimizing over ρ_0 (whose origin is again the coherent states), we obtain the desired temperature dependence of the interaction term. Furthermore, we use a box method and construct a trial state that is a tensor product of identical copies (up to translation) of the above trial state, which effectively decouples the thermodynamic limit and the dilute limit in our estimates. It should be noted that the proof of the upper bound in two dimensions is conceptually simpler than the corresponding proof of [79, Theorem 1] in three dimensions. The reason for this is based on the fact that in two dimensions it is easier to control the norm of the trial state. The error terms related to this norm being close to one are much smaller than the scale of the interaction energy, which is not the case in three dimensions. There it was critical that the terms coming from such norm estimates remain on a smaller scale than the interaction energy.

1.4 Toy model with δ interaction potential

In this section we show how to obtain an upper bound on the free energy that has the same form as the left-hand side of (1.2.20) (without the infimum). We do this by considering a toy model Hamiltonian H' with a density-dependent δ interaction potential,

$$H' = -\sum_{i=1}^{N} \Delta_i + \frac{8\pi}{|\ln a^2\rho|} \sum_{i<j}^{N} \delta(x_i - x_j) =: H_0 + V, \tag{1.4.1}$$

where in the last equality we split the Hamiltonian in the free part H_0, which contains the kinetic energy and the interacting part V. Strictly speaking, this can only be well-defined in the sense of quadratic forms on a domain of sufficiently nice functions. As we are only interested in expectation values of H' in a particular trial state (see (1.4.4) below), this shall not concern us further.

The definition of H' is motivated by perturbation theory: If we perform a first order perturbation theory for the ground state of H_0, we obtain for the change in energy

$$\frac{\Delta H}{|\Lambda|} = \frac{1}{|\Lambda|} \langle V \rangle_{H_0} = \frac{8\pi}{|\ln a^2\rho||\Lambda|^3} \sum_{i<j}^{N} \int_{\Lambda\times\Lambda} \delta(x_i - x_j)\, \mathrm{d}x_i\, \mathrm{d}x_j = \frac{4\pi\rho^2}{|\ln a^2\rho|} + o(1) \tag{1.4.2}$$

in the thermodynamic limt. Here we have used the fact that the ground state of H_0 is a (suitably normalized) constant and that its ground state energy is zero. The term obtained in the last equality above is exactly the leading order term of the ground state energy (1.1.4) in the dilute limit and therefore H' is a plausible candidate for determining an asymptotic formula for the free energy.

Denote for a density matrix $\tilde{\rho}$ the von Neumann entropy by $S(\tilde{\rho}) = -\operatorname{Tr}\tilde{\rho}\ln\tilde{\rho}$. By the Gibbs variational principle, we obtain the upper bound for the free energy (in finite volume)

$$\begin{aligned} F = -\frac{1}{\beta}\ln \operatorname{Tr} \mathrm{e}^{-\beta H'} &= \min_{\tau}\left[\operatorname{Tr} H'\tau - \frac{1}{\beta}S(\tau)\right] \\ &\leq \operatorname{Tr} H'\tilde{\rho} - \frac{1}{\beta}S(\tilde{\rho}) = \operatorname{Tr} H_0\tilde{\rho} + \operatorname{Tr} V\tilde{\rho} - \frac{1}{\beta}S(\tilde{\rho}), \end{aligned} \tag{1.4.3}$$

where the minimum is taken over all density matrices τ such that $0 \leq \tau \leq 1$, $\operatorname{Tr}\tau = 1$ as well as $\operatorname{Tr} N\tau = \rho L^2$ and the inequality holds for all $\tilde{\rho}$ satisfying the same condition. We pick $\tilde{\rho}$ to be equal to

$$\tilde{\rho} = \mathcal{D}(\lambda)^\dagger \tilde{\rho}_0^\mu \mathcal{D}(\lambda), \tag{1.4.4}$$

where $\mathcal{D}(\lambda) = \mathrm{e}^{\lambda a_0^\dagger - \lambda^* a_0}$ is the unitary coherent state operator of the $p = 0$ mode for $\lambda \in \mathbb{C}$ (with $|\lambda|^2 = \rho_0 L^2$) and $\tilde{\rho}_0^\mu$ is the grand canonical density matrix for the non-interacting system

$$\tilde{\rho}_0^\mu = \frac{1}{Z_0}\,\mathrm{e}^{-\beta(H_0-\mu N)}, \quad Z_0 = \mathrm{Tr}\,\mathrm{e}^{-\beta(H_0-\mu N)}, \tag{1.4.5}$$

where μ is chosen such that the expected number of particles in the state $\tilde{\rho}_0^\mu$ is equal to

$$\langle N\rangle_{\tilde{\rho}_0^\mu} = (\rho-\rho_0)L^2. \tag{1.4.6}$$

By a direct calculation, the expected number of particles in the state $\tilde{\rho}_0^\mu$ is given by

$$\langle N\rangle_{\tilde{\rho}_0^\mu} = Z_0^{-1} \sum_{p\in(2\pi/L)\mathbb{Z}^2} \mathrm{Tr}\, n_p\, \mathrm{e}^{-\beta(H_0-\mu N)} = \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z_0. \tag{1.4.7}$$

Here, Z_0 is the (grand canonical) partition sum of a free Bose gas, which is given by

$$\begin{aligned} Z_0 &= \mathrm{Tr}\,\mathrm{e}^{-\beta(H_0-\mu N)} \\ &= \sum_{\{n_p\}} \exp\left[-\beta \sum_{p\in(2\pi/L)\mathbb{Z}^2} \left(p^2-\mu\right) n_p\right] \\ &= \prod_p \sum_{n_p=0}^{\infty} \exp\left[-\beta\left(p^2-\mu\right)n_p\right] \\ &= \prod_p \left(1-\mathrm{e}^{-\beta(p^2-\mu)}\right)^{-1}. \end{aligned} \tag{1.4.8}$$

Thus, we have

$$\begin{aligned} (\rho-\rho_0)L^2 &= \sum_p \left(\mathrm{e}^{\beta(p^2-\mu)} - 1\right)^{-1} \\ &= \frac{L^2}{4\beta\pi}\int_0^\infty \left(\mathrm{e}^u\,\mathrm{e}^{-\beta\mu} - 1\right)^{-1}\,\mathrm{d}u + o(L^2) \\ &= -\frac{L^2}{4\beta\pi}\ln\left(1-\mathrm{e}^{\beta\mu}\right) + o(L^2), \end{aligned} \tag{1.4.9}$$

where $o(L^2)$ refers to the limit $L \to \infty$. In the calculation we used the integral

$$\int_0^\infty \left(\mathrm{e}^u\, a^{-1} - 1\right)^{-1}\,\mathrm{d}u = -\ln(1-a), \quad 0 < a < 1. \tag{1.4.10}$$

Inverting (1.4.9), we have

$$e^{\beta\mu} = 1 - e^{-4\pi\beta(\rho-\rho_0)}, \tag{1.4.11}$$

ignoring terms that give no contribution in the thermodynamic limit. Recalling our previous choice of $|\lambda|^2 = \rho_0 L^2$, we have that the state $\tilde{\rho}$ defined in (1.4.4) has an expected number of particles

$$\langle N\rangle_{\tilde{\rho}} = \operatorname{Tr} N\tilde{\rho} = \operatorname{Tr} N\mathcal{D}(\lambda)^\dagger \tilde{\rho}_0^\mu \mathcal{D}(\lambda) = |\lambda|^2 + (\rho-\rho_0)L^2 = \rho L^2, \tag{1.4.12}$$

which makes it thus an admissible trial state for the canonical Gibbs functional. Note that the right hand side of (1.4.3) can be written as

$$\operatorname{Tr} H_0\tilde{\rho} - \frac{1}{\beta}S(\tilde{\rho}) + \operatorname{Tr} V\tilde{\rho} = \operatorname{Tr} H_0\tilde{\rho}_0^\mu - \frac{1}{\beta}S(\tilde{\rho}_0^\mu) + \operatorname{Tr} V\tilde{\rho}, \tag{1.4.13}$$

where we used the fact that $\mathcal{D}$ and H_0 commute as well as the equality $S(\tilde{\rho}) = S(\tilde{\rho}_0^\mu)$. Now we note that the first two terms in the equality above constitute part of the non-interacting grand canonical Gibbs functional. In particular, if we add the term $-\mu \operatorname{Tr} N\tilde{\rho}_0^\mu$, these three terms together give exactly the free energy[2] of the non-interacting grand canonical ensemble. Therefore, we have

$$F \le \operatorname{Tr}(H_0-\mu N)\tilde{\rho}_0^\mu - \frac{1}{\beta}S(\tilde{\rho}_0^\mu) + \mu \operatorname{Tr} N\tilde{\rho}_0^\mu + \operatorname{Tr} V\tilde{\rho} = F_0 + \mu(\rho-\rho_0)L^2 + \operatorname{Tr} V\tilde{\rho}. \tag{1.4.14}$$

The first term can be evaluated explicitly as

$$\begin{aligned} F_0 &= -\frac{1}{\beta}\ln Z_0 = -\frac{1}{\beta}\ln \prod_p \sum_{n_p=0}^{\infty} e^{-\beta(p^2-\mu)n_p} \\ &= \frac{1}{\beta}\sum_p \ln\left(1 - e^{-\beta(p^2-\mu)}\right) = \frac{L^2}{4\beta^2\pi}\int_0^\infty \ln\left(1 - e^{-u}\, e^{\beta\mu}\right) du + o(L^2) \\ &= \frac{L^2}{4\beta^2\pi}\int_0^\infty \ln\left(1 - e^{-u}\left(1 - e^{-4\pi\beta(\rho-\rho_0)}\right)\right) du + o(L^2), \end{aligned} \tag{1.4.15}$$

[2]Actually, if we consider the three terms

$$\operatorname{Tr}(H_0-\mu N)\tilde{\rho}_0^\mu - \frac{1}{\beta}S(\tilde{\rho}_0^\mu)$$

as a function of β and μ this is nothing else but the grand canonical pressure functional of $\tilde{\rho}_0^\mu$ (up to an area factor) for the non-interacting system. Since we insert the value of the chemical potential from (1.4.11), we effectively perform the Legendre transform and end up with the free energy.

where we inserted in the last equality the value of the chemical potential from (1.4.11) needed to achieve an expected number of particles $(\rho - \rho_0)L^2$ in the state $\tilde{\rho}_0^\mu$.

Let us discuss the evaluation of the term $\langle V \rangle_{\tilde{\rho}}$. We consider general states in Fock space of the form

$$|n_\lambda\rangle = |\lambda, n_0, n_1, \dots\rangle = C_n \, e^{-|\lambda|^2/2} \left[e^{\lambda a_0^\dagger} (a_0^\dagger)^{n_0} (a_1^\dagger)^{n_1} \cdots \right] |\text{vac}\rangle \,. \tag{1.4.16}$$

In second quantization, we can write the expectation value of the δ potential for a many-body wave function Φ in the following way

$$\sum_{i<j} \langle \Phi, \delta(x_i - x_j)\Phi\rangle = \frac{1}{2L^2} \sum_{\alpha,\beta,\gamma,\delta} \delta_{\alpha+\beta,\gamma+\delta} \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta | n_\lambda \rangle \tag{1.4.17}$$

and by a direct calculation, we obtain for the Fock space expectation (using the fact that $a_0 \, e^{\lambda a_0^\dagger} = e^{\lambda a_0^\dagger}(\lambda + a_0)$)

$$\begin{aligned}
&\langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta | n_\lambda\rangle = \delta_{\delta 0}\lambda \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger a_\gamma | n_\lambda \rangle + \sqrt{n_\delta} \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger a_\gamma | n_\delta - 1, \lambda\rangle \\
&= \delta_{\delta 0}\lambda \left[\delta_{\gamma 0}\lambda \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger | n_\lambda\rangle + \sqrt{n_\gamma} \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger | n_\gamma - 1, \lambda \rangle \right] \\
&\quad + \sqrt{n_\delta} \Big[\delta_{\gamma 0}\lambda \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger | n_\delta - 1, \lambda\rangle \\
&\quad + \delta_{\gamma\delta} \sqrt{n_\delta - 1} \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger | n_\delta - 2, \lambda \rangle \\
&\quad + (1 - \delta_{\gamma\delta}) \sqrt{n_\gamma} \, \langle n_\lambda | a_\alpha^\dagger a_\beta^\dagger | n_\delta - 1, n_\gamma - 1, \lambda \rangle \Big] \\
&= \delta_{\delta 0}\delta_{\gamma 0}\delta_{\alpha 0}\delta_{\beta 0}|\lambda|^4 + \delta_{\delta 0}\lambda \sqrt{n_\gamma} \left[\delta_{\beta 0}\lambda^* \delta_{\alpha\gamma} \sqrt{n_\gamma} + \delta_{\alpha 0}\lambda^*\delta_{\beta\gamma} \sqrt{n_\gamma} \right] \\
&\quad + \sqrt{n_\delta}\delta_{\gamma 0}\lambda \left[\delta_{\beta 0}\lambda^*\delta_{\alpha\delta}\sqrt{n_\delta} + \delta_{\alpha 0}\lambda^*\delta_{\beta\delta}\sqrt{n_\delta} \right] \\
&\quad + \sqrt{n_\delta}\delta_{\gamma\delta}\sqrt{n_\delta - 1}\delta_{\beta\delta}\delta_{\alpha\delta}\sqrt{n_\delta - 1}\sqrt{n_\delta} \\
&\quad + (1 - \delta_{\gamma\delta})\sqrt{n_\delta}\sqrt{n_\gamma} \left[\delta_{\beta\delta}\delta_{\alpha\gamma}\sqrt{n_\delta}\sqrt{n_\gamma} + \delta_{\beta\gamma}\delta_{\alpha\delta}\sqrt{n_\delta}\sqrt{n_\gamma} \right] \\
&= \delta_{\delta 0}\delta_{\gamma 0}\delta_{\alpha 0}\delta_{\beta 0}|\lambda|^4 + \delta_{\delta 0}|\lambda|^2 n_\gamma \left[\delta_{\beta 0}\delta_{\alpha\gamma} + \delta_{\alpha 0}\delta_{\beta\gamma} \right] \\
&\quad + \delta_{\gamma 0}|\lambda|^2 n_\delta \left[\delta_{\beta 0}\delta_{\alpha\delta} + \delta_{\alpha 0}\delta_{\beta\delta} \right] \\
&\quad + \delta_{\gamma\delta}\delta_{\beta\delta}\delta_{\alpha\delta} n_\delta (n_\delta - 1) \\
&\quad + (1 - \delta_{\gamma\delta}) n_\delta n_\gamma \left[\delta_{\beta\delta}\delta_{\alpha\gamma} + \delta_{\beta\gamma}\delta_{\alpha\delta} \right] \\
&= \delta_{\delta 0}\delta_{\gamma 0}\delta_{\alpha 0}\delta_{\beta 0}|\lambda|^4 + 4\delta_{\alpha\gamma}\delta_{\beta 0}\delta_{\delta 0}|\lambda|^2 n_\alpha \\
&\quad + \delta_{\alpha\beta}\delta_{\alpha\gamma}\delta_{\alpha\delta} n_\alpha (n_\alpha - 1) \\
&\quad + 2\delta_{\alpha\gamma}\delta_{\beta\delta}(1 - \delta_{\gamma\delta}) n_\delta n_\gamma .
\end{aligned} \tag{1.4.18}$$

Statistical averaging with respect to the state $\tilde{\rho}$ gives (setting $|\lambda|^2 = \mathcal{N}_0 = \rho_0 L^2$)

$$\begin{aligned}
\langle V\rangle_{\tilde{\rho}} &= \frac{8\pi}{|\ln a^2\rho|L^2}\left(\frac{1}{2}|\lambda|^4 + 2|\lambda|^2\sum_p \langle n_p\rangle_{\tilde{\rho}_0^\mu} + \frac{1}{2}\sum_p \langle n_p(n_p-1)\rangle_{\tilde{\rho}_0^\mu} + \sum_{p\neq k}\langle n_p n_k\rangle_{\tilde{\rho}_0^\mu}\right)\\
&= \frac{8\pi}{|\ln a^2\rho|L^2}\left(\frac{1}{2}\mathcal{N}_0^2 + (2\mathcal{N}_0 - 1/2)\mathcal{N}_> - \frac{1}{2}\sum_p \langle n_p^2\rangle_{\tilde{\rho}_0^\mu} + \mathcal{N}_>^2\right)\\
&= \frac{8\pi}{|\ln a^2\rho|L^2}\left(\mathcal{N}_>^2 + \frac{1}{2}\mathcal{N}_0^2 + (2\mathcal{N}_0 - 1)\mathcal{N}_> + r\right)\\
&= \frac{8\pi}{|\ln a^2\rho|L^2}\left((\rho-\rho_0)^2L^4 + \frac{1}{2}\rho_0^2L^4 + 2\rho_0L^2(\rho-\rho_0)L^2 - (\rho-\rho_0)L^2 + r\right)\\
&= \frac{8\pi L^2}{|\ln a^2\rho|}\left(\rho^2 - \frac{1}{2}\rho_0^2 - \frac{\rho-\rho_0}{L^2} + \frac{r}{L^4}\right),
\end{aligned}\tag{1.4.19}$$

where r is a correction term. Explicitly, r is given by $r = 1 - e^{4\pi\beta(\rho-\rho_0)}$ and it is clear that it gives no contribution in the limit $L \to \infty$ as it comes with a factor of L^{-4}. Suppressing the terms of lower order, we thus obtain the result

$$\langle V\rangle_{\tilde{\rho}} = \frac{8\pi L^2}{|\ln a^2\rho|}\left(\rho^2 - \frac{1}{2}\rho_0^2\right) = \frac{8\pi L^2}{|\ln a^2\rho|}\rho^2\left(1 - \frac{\rho_0^2}{2\rho^2}\right). \tag{1.4.20}$$

Alternatively, this result could have been obtained by writing $\langle V\rangle_{\tilde{\rho}} = \langle \mathcal{D}(\lambda)V\mathcal{D}(\lambda)^\dagger\rangle_{\tilde{\rho}_0^\mu}$. Using the fact that the coherent state operator acts as a shift operator on the $p = 0$ mode creation/annihilation operators, i.e., we have

$$\mathcal{D}(\lambda)a_0\mathcal{D}(\lambda)^\dagger = a_0 + \lambda \tag{1.4.21}$$

and its conjugate, we get

$$\begin{aligned}
\sum_{i<j}\langle \delta(x_i - x_j)\rangle_{\tilde{\rho}} &= \frac{1}{2L^2}\sum_{\alpha,\beta,\gamma,\delta}\delta_{\alpha+\beta,\gamma+\delta}\,\langle \mathcal{D}(\lambda)a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \mathcal{D}(\lambda)^\dagger\rangle_{\tilde{\rho}_0^\mu}\\
&= \frac{1}{2L^2}\sum_{\alpha,\beta,\gamma,\delta}\delta_{\alpha+\beta,\gamma+\delta}\,\langle (a_\alpha^\dagger + \lambda^*)(a_\beta^\dagger + \lambda^*)(a_\gamma + \lambda)(a_\delta + \lambda)\rangle_{\tilde{\rho}_0^\mu}\,.
\end{aligned}\tag{1.4.22}$$

Since the state $\tilde{\rho}_0^\mu$ is quasi-free and particle number conserving, we can apply Wick's rule to obtain the result (1.4.20).

Combining both the expression for the free energy of the free Bose gas from (1.4.15) and the result for the expectation of the δ interaction from (1.4.20) and dividing by L^2, we have the following upper bound to the free energy per unit volume of the Hamiltonian with δ interaction. Denoting the quasi-condensate fraction by $s = \rho_0/\rho$, the bound takes the form

$$f \le 4\pi\rho^2 \left[\frac{1}{(4\pi\beta\rho)^2} \int_0^\infty \ln\left(1 - \mathrm{e}^{-u}\left(1 - \mathrm{e}^{-4\pi\beta\rho(1-s)}\right)\right) \mathrm{d}u \right.$$
$$\left. + \frac{1-s}{4\pi\beta\rho} \ln\left(1 - \mathrm{e}^{-4\pi\beta\rho(1-s)}\right) + \frac{1}{|\ln a^2\rho|}\left(2 - s^2\right)\right], \tag{1.4.23}$$

where we suppressed the terms that vanish in the thermodynamic limit.

1.5 Minimizing over the quasi-condensate fraction

In this section we show how to obtain the right-hand side of (1.2.20) to leading order in the dilute limit. Recall that we obtained the left-hand side of (1.2.20) (without the infimum) as the result of the previous Section 1.4, i.e.,

$$f_0(\beta, \rho(1-s)) + \frac{4\pi\rho^2}{|\ln a^2\rho|}\left(2 - s^2\right) = \text{right-hand side of (1.4.23)} \tag{1.5.1}$$

for $s = \rho_0/\rho$. Based on the different monotonicity of the free energy and the interaction term on the left-hand side in (1.5.1) it is possible to guess that there is a non-trivial (i.e., not zero or one) optimum when minimizing over s. Indeed, the result of the minimization in Lemma 1 below is (to leading order)

$$\rho_{\mathrm{s}} = \rho\left[1 - \frac{\ln|\ln a^2\rho|}{4\pi\beta\rho}\right]_+ = \rho\left[1 - \frac{\beta_{\mathrm{c}}}{\beta}\right]_+, \tag{1.5.2}$$

where we recall that the inverse critical temperature was defined in (1.1.7) as $\beta_{\mathrm{c}} = \frac{\ln|\ln a^2\rho|}{4\pi\rho}$ and $[\,\cdot\,]_+ = \max\{0, \cdot\}$ denotes the positive part.

Introducing the function

$$g_s(\epsilon, \lambda) := \frac{1}{\ln^2\epsilon} \int_0^\infty \ln\left(1 - \mathrm{e}^{-u}\left(1 - \epsilon^{1-s}\right)\right) \mathrm{d}u - \frac{1-s}{\ln\epsilon} \ln\left(1 - \epsilon^{1-s}\right) + \lambda\left(2 - s^2\right), \tag{1.5.3}$$

we have that $g_s(\epsilon, \lambda)$ with $\epsilon = \mathrm{e}^{-4\pi\beta\rho}$ and $\lambda = 1/|\ln a^2\rho|$ is equal (up to a factor of $4\pi\rho^2$) to the left-hand side of (1.5.1). When minimizing $g_s(\epsilon, \lambda)$ over $s \in [0, 1]$ we thus obtain the best upper bound for the leading order term. Note that using the series expansion of the logarithm, g_s can be rewritten as

$$g_s(\epsilon, \lambda) = -\frac{1}{\ln^2\epsilon} \mathrm{Li}_2(1 - \epsilon^{1-s}) - \frac{1-s}{\ln\epsilon} \ln(1 - \epsilon^{1-s}) + \lambda(2 - s^2), \tag{1.5.4}$$

where $\mathrm{Li}_n(z)$ is the polylogarithm defined by

$$\mathrm{Li}_n(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^n} \tag{1.5.5}$$

and for $n = 2$ it can also be written as

$$\mathrm{Li}_2(z) = -\int_0^z \frac{\ln(1-t)}{t}\,\mathrm{d}t. \tag{1.5.6}$$

We have the following lemma about the minimum of the function $g_s(\epsilon, \lambda)$.

Lemma 1. *In the region $\mathcal{L} = \{(\epsilon, \lambda) : \lambda \leq \epsilon\}$, the function $g_s(\epsilon, \lambda)$ defined by* (1.5.3) *is minimized at $s = 0$ with minimal value*

$$g_0(\epsilon, \lambda) = g_0(\epsilon, 0) + 2\lambda. \tag{1.5.7}$$

In the region $\mathcal{U} = \{(\epsilon, \lambda) : \lambda > \epsilon\}$ we have a statement only in the limit $\lambda \to 0$ (which means that also $\epsilon \to 0$ since we are in a region where $\epsilon < \lambda$). We have that $g_s(\epsilon, \lambda)$ is minimized at $s_{min} = 1 - \ln\lambda / \ln\epsilon + o(1) > 0$ with minimal value

$$g_{s_{min}}(\epsilon, \lambda) = g_0(\epsilon, 0) + \lambda\left(2 - \left(1 - \frac{\ln\lambda}{\ln\epsilon}\right)^2\right) + o(\lambda) \tag{1.5.8}$$

as $\lambda \to 0$. Combining the two cases $\lambda \leq \epsilon$ and $\lambda > \epsilon$ into a single formula, we write $\lambda = \epsilon^{\varkappa}$ for any $0 < \varkappa < \infty$ and have that the minimum of g_s is given by

$$\min_{0 \leq s \leq 1} g_s(\epsilon, \epsilon^{\varkappa}) = g_0(\epsilon, 0) + \epsilon^{\varkappa}(2 - [1 - \varkappa]_+^2) + o(\epsilon^{\varkappa}) \tag{1.5.9}$$

as $\epsilon \to 0$. Here, $[\,\cdot\,]_+$ denotes the positive part.

Proof. Parametrize a point p in $\mathcal{L} = \{\lambda \leq \epsilon\}$ as $p = (\epsilon, \epsilon^{\varkappa})$ with $\varkappa \geq 1$ and $0 \leq \epsilon \leq 1$. Then we show that $g_s(\epsilon, \epsilon^{\varkappa})$ is a strictly increasing function in s and therefore attains the minimum at $s = 0$. In other words, we should show

$$\frac{\partial}{\partial s} g_s(\epsilon, \epsilon^{\varkappa}) = \frac{\ln(1 - \epsilon^{1-s})}{\ln\epsilon} - 2s\epsilon^{\varkappa} > 0. \tag{1.5.10}$$

Using the inequality $\ln(1 - x) \leq -x$ for $x < 1$, it is enough to show

$$-\epsilon^{\varkappa+s-1}\ln\epsilon < \frac{1}{2s} \tag{1.5.11}$$

to obtain (1.5.10). An explicit calculation shows that the function $\epsilon \mapsto -\epsilon^{\alpha} \ln \epsilon$ is maximized at $1/(\alpha\,\mathrm{e})$ and thus we have, plugging in $\alpha = \varkappa + s - 1$,

$$-\epsilon^{\varkappa+1-s} \ln \epsilon \leq \frac{1}{(\varkappa + s - 1)\,\mathrm{e}} \leq \frac{1}{\mathrm{e}\, s} < \frac{1}{2s} \tag{1.5.12}$$

which proves that $g_s(\epsilon, \epsilon^{\varkappa})$ is strictly increasing in s and that the minimum is attained at $s = 0$ in the case $\varkappa \geq 1$.

To minimize g_s in the region $\mathcal{U} = \{\lambda > \epsilon\}$, we first note that the partial derivative of g_s with respect to s,

$$\frac{\partial}{\partial s} g_s(\epsilon, \lambda) := h(s) = \frac{\ln(1 - \epsilon^{1-s})}{\ln \epsilon} - 2\lambda s, \tag{1.5.13}$$

is a convex function of s. This can be easily checked by computing the second derivative of $h(s)$, which is indeed positive for $0 < \epsilon < 1$:

$$h''(s) = -\ln \epsilon \frac{\epsilon^{s+1}}{(\epsilon - \epsilon^{s})^2} > 0 \tag{1.5.14}$$

Thus we deduce that the equation $h(s) = 0$ has at most two solutions. Since $h(0) > 0$, the first zero (counting from the left) of h is a maximum of g_s, while the second zero is a minimum of g_s. The equation $h(s) = 0$ can be rewritten (by taking the logarithm) for $\lambda = \epsilon^{\varkappa}$ with $0 < \varkappa < 1$ as

$$s = 1 - \varkappa - \frac{\ln(2s|\ln \epsilon|)}{\ln \epsilon}. \tag{1.5.15}$$

By examination, one sees that this equation can have up to two solutions: As it is of the form $s = a + b \ln s$, we see that the line through the origin with slope one can intersect up to two times with the shifted logarithm. If it has in fact two solutions, we are looking for the second solution away from zero in the sense that $\ln s$ stays bounded as $\epsilon \to 0$. But then we have already found the solution approximately, since we have

$$s_{\min} = 1 - \varkappa + O\left(\frac{\ln|\ln \epsilon|}{|\ln \epsilon|}\right). \tag{1.5.16}$$

Inserting this into g_s, we find

$$\begin{aligned} g_{s_{\min}}(\epsilon, \epsilon^{\varkappa}) &= g_{s_{\min}}(\epsilon, 0) + \epsilon^{\varkappa}(2 - s_{\min}^2) \\ &= g_{s_{\min}}(\epsilon, 0) + \epsilon^{\varkappa}(2 - (1-\varkappa)^2) + O\left(\epsilon^{\varkappa}\left(\frac{\ln|\ln \epsilon|}{|\ln \epsilon|}\right)^2\right). \end{aligned} \tag{1.5.17}$$

It remains to check that the error we make by replacing $g_{s_{\min}}(\epsilon, 0)$ by $g_0(\epsilon, 0)$ is of lower order than the error term we have already written. We have

$$\begin{aligned} g_{s_{\min}}(\epsilon, 0) &= -\frac{1}{\ln^2 \epsilon} \operatorname{Li}_2(1 - \epsilon^{1-s_{\min}}) - \frac{1 - s_{\min}}{\ln \epsilon} \ln(1 - \epsilon^{1-s_{\min}}) \\ &= -\frac{1}{\ln^2 \epsilon} \left(\frac{\pi^2}{6} + (\ln \epsilon^{1-s_{\min}} - 1)\epsilon^{1-s_{\min}} \right) + \frac{1 - s_{\min}}{\ln \epsilon} \epsilon^{1-s_{\min}} + O\left(\frac{\epsilon^{2(1-s_{\min})}}{|\ln \epsilon|} \right) \\ &= -\frac{1}{\ln^2 \epsilon} \left(\frac{\pi^2}{6} - \epsilon^{1-s_{\min}} \right) + O\left(\frac{\epsilon^{2(1-s_{\min})}}{|\ln \epsilon|} \right). \end{aligned} \tag{1.5.18}$$

For $g_0(\epsilon, 0)$ we find similarly

$$g_0(\epsilon, 0) = -\frac{1}{\ln^2 \epsilon} \left(\frac{\pi^2}{6} - \epsilon \right) + O\left(\frac{\epsilon^2}{|\ln \epsilon|} \right). \tag{1.5.19}$$

Therefore, we find that in the difference of $g_{s_{\min}}(\epsilon, 0)$ and $g_0(\epsilon, 0)$ the leading order term proportional to $1/\ln^2 \epsilon$ cancels. The next order term in the expansion for $g_{s_{\min}}(\epsilon, 0)$ proportional to $\epsilon^{1-s_{\min}}/\ln^2 \epsilon$ is much bigger than the next order term in the expansion for $g_0(\epsilon, 0)$ and in conclusion we have

$$\begin{aligned} g_{s_{\min}}(\epsilon, 0) - g_0(\epsilon, 0) &= \frac{\epsilon^{1-s_{\min}}}{\ln^2 \epsilon} + O\left(\max\left\{ \frac{\epsilon^{2(1-s_{\min})}}{|\ln \epsilon|}, \frac{\epsilon}{\ln^2 \epsilon} \right\} \right) \\ &= O\left(\frac{\epsilon^{\varkappa}}{\ln^2 \epsilon} \right). \end{aligned} \tag{1.5.20}$$

Thus, we can replace $g_{s_{\min}}(\epsilon, 0)$ by $g_0(\epsilon, 0)$ in (1.5.17) and obtain

$$g_{s_{\min}}(\epsilon, \epsilon^{\varkappa}) = g_0(\epsilon, 0) + \epsilon^{\varkappa}(2 - (1 - \varkappa)^2) + O\left(\epsilon^{\varkappa} \left(\frac{\ln|\ln \epsilon|}{|\ln \epsilon|} \right)^2 \right). \tag{1.5.21}$$

Finally, we combine both cases, $0 < \varkappa < 1$ and $\varkappa \geq 1$, into a single formula

$$g_{s_{\min}}(\epsilon, \epsilon^{\varkappa}) = g_0(\epsilon, 0) + \epsilon^{\varkappa}(2 - [1 - \varkappa]_+^2) + O\left(\epsilon^{\varkappa} \left(\frac{\ln|\ln \epsilon|}{|\ln \epsilon|} \right)^2 \right). \tag{1.5.22}$$

Now we are done, since the error term in (1.5.22) is indeed $o(\epsilon^{\varkappa})$ (albeit with a very slow convergence rate). □

See Figure 1.1 for a numerical evaluation of the statement of Lemma 1. One recognizes the exact minimum $s = 0$ in the lower region $\mathcal{L}$ as well as the approximate minimum $s_{\min} = 1 - \varkappa$ in the upper region $\mathcal{U}$. In the upper bound in Chapter 3 below, we therefore directly work with a trial state that has density ρ_s in the coherent state of the $p = 0$ mode.

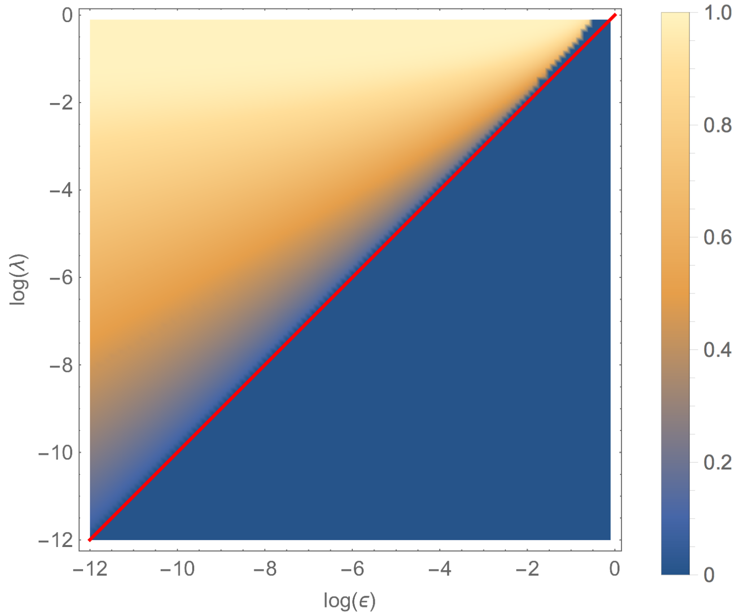

Figure 1.1: The color marks the numerically determined position s of the minimum of $g_s(\epsilon, \lambda)$ in the (ϵ, λ)-plane on a doubly logarithmic scale. The red line is $\ln \lambda = \ln \epsilon$.

1.6 The finite potential well in two dimensions: ground state energy and scattering length

In Lemma 5 in Section 2.9 below we will prove an inequality for a one-body Schrödinger operator with a finite potential well. The method used in the proof is quite general and uses [74, Theorem 3.4] about the scaling behavior (for a small coupling constant) of the ground state energy of Schrödinger operators. In this section we will see that for the finite potential well it is possible to obtain the scaling behavior of the ground state energy (as well as the scattering length) in a shorter and more direct way using some algebra and physical intuition.

We consider for $\lambda > 0$ the Hamiltonian

$$h = -\Delta - \lambda \theta(R_0 - |x|) \tag{1.6.1}$$

acting on $L^2(\mathbb{R}^2)$, which describes a single particle interacting with an attractive potential well of radius R_0 and coupling strength λ. Our goal is to obtain the scaling behavior of the ground state energy as well as the scattering length. The stationary Schrödinger equation at energy E in polar coordinates reads

$$\left(-\frac{\partial^2}{\partial r^2} - \frac{1}{r}\frac{\partial}{\partial r} - \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} - \lambda\theta(R_0 - r)\right)\psi(r,\varphi) = E\psi(r,\varphi). \tag{1.6.2}$$

By separation of variables and solving the equation for the angular variable, we find the ODE

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} + \frac{m^2}{r^2} - E - \lambda\theta(R_0 - r)\right)R(r) = 0 \tag{1.6.3}$$

for m an integer. Rescaling $\rho = r\sqrt{E + \lambda\theta(R_0 - r)}$ leads to the equation

$$\left(\rho^2\frac{\mathrm{d}^2}{\mathrm{d}\rho^2} + \rho\frac{\mathrm{d}}{\mathrm{d}\rho} + \rho^2 - m^2\right)R(\rho) = 0, \tag{1.6.4}$$

which is Bessel's equation for $R(\rho)$. Strictly speaking we have two equations, one for $r < R_0$ and one for $r > R_0$ (since the rescaling we did was discontinuous), and we have to patch together the solutions in a suitable way (by matching the solutions and their derivatives). To find the ground state energy we can assume $m = 0$ (as the ground state wave function will have no angular momentum). Denoting

$$k = \sqrt{\lambda - |E|}, \quad \varkappa = \sqrt{|E|}, \tag{1.6.5}$$

we solve (1.6.4) by

$$R(\rho) \sim \begin{cases} J_0(kr) & \text{if } 0 \le r < R_0, \\ K_0(\varkappa r) & \text{if } r > R_0. \end{cases} \tag{1.6.6}$$

Here, J_0 is the Bessel function of the first kind and K_0 is the modified Bessel function of the second kind. This ansatz is regular inside the potential well and decays exponentially outside, as is appropriate for a bound state with $E < 0$. Matching the two functions and their derivatives at $r = R_0$ (as well as eliminating the normalization factor) leads to the equation

$$k\frac{J_0'(kR_0)}{J_0(kR_0)} = \varkappa\frac{K_0'(\varkappa R_0)}{K_0(\varkappa R_0)}. \tag{1.6.7}$$

The smallest E that solves (1.6.7) is then the ground state energy E_0 that we are searching for. Since we are only interested in the scaling behavior of E_0 for small λ (which means $E_0 \to 0$), we can insert the asymptotic form of the Bessel functions around zero into this equation. We have[3], as $x \to 0$,

$$J_0(x) \approx 1 - \frac{x^2}{4}, \qquad J_0'(x) \approx -\frac{x}{2},$$
$$K_0(x) \approx -\ln x, \qquad K_0'(x) \approx -\frac{1}{x}. \tag{1.6.8}$$

Therefore, the asymptotic form of (1.6.7) is

$$-\frac{R_0^2}{2}(\lambda - |E_0|) = \frac{1}{\ln(\sqrt{|E_0|}R_0)}, \tag{1.6.9}$$

which is equivalent to

$$|E_0| - \frac{4}{R_0^2 \ln(|E_0|R_0^2)} = \lambda. \tag{1.6.10}$$

We solve it to leading order by

$$E_0 = -\frac{1}{R_0^2}\exp\left(-\frac{4}{\lambda R_0^2}\right). \tag{1.6.11}$$

To determine the scattering length of this potential we have to search for solutions of (1.6.4) with $E > 0$ (so called scattering solutions). For this purpose we need to introduce the concept of s-wave scattering (see, for example, [76]).

The general solution to (1.6.4) outside the range of the potential for any angular momentum m is a superposition of the two linearly independent solutions J_m and Y_m (which is the Bessel function of the second kind):

$$R_m(\rho) \sim A_m J_m(\sqrt{E}r) + B_m Y_m(\sqrt{E}r). \tag{1.6.12}$$

Rewriting $A_m = a_m \cos\delta_m$ and $B_m = -a_m \sin\delta_m$, with δ_m the phase shift, we have

$$R_m(\rho) \sim a_m\left(\cos\delta_m J_m(\sqrt{E}r) - \sin\delta_m Y_m(\sqrt{E}r)\right) \sim J_m(\sqrt{E}r) - \tan\delta_m Y_m(\sqrt{E}r). \tag{1.6.13}$$

This definition of δ_m can be understood in the following way. The only difference between the scattered wave and the free particle is a phase $e^{i\delta_m}$. In the low-energy limit, only the $m = 0$ contribution to the whole scattering process matters, which is called s-wave scattering. From [35], we obtain the relation between the s-wave phase shift δ_0 and the scattering length as

$$a = \lim_{E\to 0}\frac{2}{\sqrt{E}}\exp\left(\frac{\pi}{2\tan\delta_0} - \gamma\right), \tag{1.6.14}$$

[3]See, for example, [1] for the asymptotic form of the Bessel functions for small arguments.

where $\gamma \approx 0.577$ is the Euler–Mascheroni constant.

To obtain the s-wave phase shift δ_0, we have to search for solutions of (1.6.4) with $E > 0$. We denote

$$k = \sqrt{\lambda + E}, \quad \varkappa = \sqrt{E} \tag{1.6.15}$$

and propose the ansatz

$$R(\rho) \sim \begin{cases} J_0(kr) & \text{if } 0 \leq r < R_0, \\ J_0(\varkappa r) + B/A Y_0(\varkappa r) & \text{if } r > R_0. \end{cases} \tag{1.6.16}$$

Inside the range of the potential we use again a regular function and discard Y_0, while outside the range we have to superpose the two linearly independent solutions J_0 and Y_0 with coefficients A and B and have only retained the ratio between the two. As before, we have to patch together the solutions and their derivatives at $r = R_0$. This leads to

$$\varkappa \frac{AJ_1(\varkappa R_0) + BY_1(\varkappa R_0)}{AJ_0(\varkappa R_0) + BY_0(\varkappa R_0)} = k \frac{J_1(kR_0)}{J_0(kR_0)}. \tag{1.6.17}$$

This implies

$$\frac{B}{A} = \frac{\varkappa J_1(\varkappa R_0) J_0(kR_0) - kJ_0(\varkappa R_0) J_1(kR_0)}{kJ_1(kR_0) Y_0(\varkappa R_0) - \varkappa Y_1(\varkappa R_0) J_0(kR_0)}, \tag{1.6.18}$$

which allows us to eliminate the ratio B/A from (1.6.16). We can now rewrite the solution $R(\rho)$ for $r > R_0$ in the desired form to read off the s-wave phase shift as

$$R(\rho) \sim J_0(\varkappa r) - \tan\delta_0 Y_0(\varkappa r), \tag{1.6.19}$$

where

$$\tan\delta_0 = \frac{kJ_0(\varkappa R_0) J_1(kR_0) - \varkappa J_1(\varkappa R_0) J_0(kR_0)}{kJ_1(kR_0) Y_0(\varkappa R_0) - \varkappa Y_1(\varkappa R_0) J_0(kR_0)}. \tag{1.6.20}$$

Expanding this for small E and plugging back the values of k and $\varkappa$ from (1.6.15), we obtain for the s-wave phase shift

$$\tan\delta_0 = \frac{\pi}{2} \left(\ln\left(\frac{\sqrt{E} R_0}{2} \right) + \gamma + \frac{J_0(\sqrt{\lambda + E} R_0)}{\sqrt{\lambda + E} R_0 J_1(\sqrt{\lambda + E} R_0)} \right)^{-1}, \tag{1.6.21}$$

Inserting this into (1.6.14), we obtain for the scattering length of the finite potential well

$$a = \lim_{E \to 0} \frac{2}{\sqrt{E}} \exp\left(\frac{\pi}{2 \tan\delta_0} - \gamma \right) = R_0 \exp\left(\frac{J_0(\sqrt{\lambda} R_0)}{\sqrt{\lambda} R_0 J_1(\sqrt{\lambda} R_0)} \right). \tag{1.6.22}$$

Note that into this formula one can also plug negative values of λ and by analytic continuation obtain the scattering length for a repulsive potential as well.

For the special case of a logarithmic scaling of the coupling strength that we will need later in the proof of Lemma 5 in Section 2.9,

$$\lambda = \frac{1}{R_0^2 \ln(R/R_0)}, \tag{1.6.23}$$

for R such that $R/R_0 \to \infty$, we obtain for the ground state energy and the scattering length

$$E_0 \sim -\frac{1}{R^2}\left(\frac{R_0}{R}\right)^2, \quad a \sim R\left(\frac{R_0}{R}\right)^3. \tag{1.6.24}$$

The scaling behavior of E_0 is indeed (up to an ϵ in the exponent) the same as in (2.9.12).

1.7 Important differences between the two- and three-dimensional system

In this section we list some of the apparent differences between the two- and three-dimensional system. Perhaps the most important one is the size of the interaction term for the ground state energy. In contrast to three dimensions, it is not given by $N(N-1)/2$ times the energy of two particles, but is much larger. As remarked in [46, Chapter 3], to obtain the correct logarithmic factor one has to replace L, the linear size of the system (which goes to ∞ in the thermodynamic limit), by $\rho^{-1/2}$, the average distance between particles.

The next difference lies in the solution to the zero-energy scattering equation. In three dimensions that solution is given asymptotically by $g_0(r) = 1 - a/r$ with boundary condition 1 at ∞, while for the two-dimensional equation we have the asymptotic solution $g_0(r) = \ln(r/a)/\ln(R/a)$ with boundary condition 1 at $r = R$. The parameter R has to be introduced since g_0 grows logarithmically and is not normalizable on the full space. Therefore, g_0 can only be well-defined in a finite area. In the proof of the main theorem below, we will see that

$$\frac{1}{\ln(R/a)} \sim \frac{1}{|\ln a^2\rho|}, \tag{1.7.1}$$

which means that up to logarithmic corrections R has to be chosen proportional to the average particle distance $\rho^{-1/2}$.

Finally, we remark on the difference between the critical temperature that was found in Section 1.5 and the critical temperature in the three-dimensional setting. Their inverses are

$$\beta_{\mathrm{c}}^{\mathrm{3D}} = \frac{\zeta(3/2)^{2/3}}{4\pi\rho^{2/3}}, \qquad \beta_{\mathrm{c}}^{\mathrm{2D}} = \frac{\ln|\ln a^2\rho|}{4\pi\rho}. \tag{1.7.2}$$

We note that $\beta_{\mathrm{c}}^{\mathrm{3D}}$ is the inverse critical temperature for Bose–Einstein condensation of the ideal gas, which would be equal to ∞ in the two-dimensional setting. Additionally, the inverse critical temperature for superfluidity $\beta_{\mathrm{c}}^{\mathrm{2D}}$ depends directly on the interaction and is *not* related to the non-interacting system.

2 Lower bound on the free energy

Andreas Deuchert, Simon Mayer and Robert Seiringer

We prove a lower bound on the free energy of an interacting two-dimensional Bose gas in a homogeneous, dilute setting in the thermodynamic limit. We show that the free energy differs from the free energy of the non-interacting system by a correction term $4\pi\rho^2 |\ln a^2\rho|^{-1}(2 - [1 - \beta_c/\beta]_+^2)$, where a is the scattering length of the interaction potential, ρ is the density, β is the inverse temperature and β_c is the inverse critical Kosterlitz–Thouless temperature for superfluidity. The result becomes useful in the dilute limit $a^2\rho \to 0$ and if the dimensionless parameter $\beta\rho$ is of order one or larger.

2.1 Statement of the lower bound

Theorem 2 (Lower bound on the free energy)**.** *Assume that the interaction potential satisfies* $v \geq 0$ *and has a finite scattering length. As* $a^2\rho \to 0$ *with* $\beta\rho \gtrsim 1$*, we have*

$$f(\beta,\rho) \geq f_0(\beta,\rho) + \frac{4\pi\rho^2}{|\ln a^2\rho|}\left(2 - \left[1 - \frac{\beta_\mathrm{c}}{\beta}\right]_+^2\right)(1 - o(1)), \tag{2.1.1}$$

where

$$o(1) \lesssim \frac{\ln\ln|\ln a^2\rho|}{\ln|\ln a^2\rho|}. \tag{2.1.2}$$

Here, $[\,\cdot\,]_+ = \max\{\,\cdot\,,0\}$ *denotes the positive part and the inverse critical temperature* $\beta_\mathrm{c}(\rho,a)$ *is defined in* (1.1.7).

2.2 Sketch of the proof

A key ingredient in the proof of the lower bound on the free energy of the interacting gas is the observation that the second term on the right-hand side of (2.1.1) (the interaction energy) is, in the dilute limit, much smaller than the first term $f_0(\beta,\rho)$. As remarked above (in Section 1.2), a naive version of first order perturbation theory fails, however, for two reasons. First, the interaction potential is so strong that the interaction energy of the Gibbs state of the ideal gas is too large (it is even infinite in the case of hard disks). Secondly, the temperature dependence of the interaction term comes out wrong, as $\rho[1-\beta_\mathrm{c}/\beta]_+$ depends on the scattering length, which clearly cannot be captured by an ideal gas state.

The first problem is overcome with the aid of a version of the Dyson Lemma [23]. This Lemma allows to replace the strong interaction potential v by a softer potential with a longer range that can later be treated using a rigorous version of first order perturbation theory. The price one has to pay is a certain amount of the kinetic energy. It is important that only modes with momenta much larger than $\beta^{-1/2}$ are used in this procedure because the other modes are needed to build up the free energy $f_0(\beta,\rho)$ of the ideal gas. A version of the Dyson Lemma fulfilling such requirements was for the first time proved in [45] to treat the ground state energy of the dilute Fermi gas.

After this replacement we utilize a rigorous version of first order perturbation theory at positive temperature, which was developed in [70]. The method is based on a correlation inequality [68] that applies to fermionic systems at all temperatures and to bosonic systems at sufficiently large temperatures. The main ingredient needed for this method to work is that the reference state in the perturbative analysis (usually the Gibbs state of the corresponding ideal gas) shows an approximate tensor product structure with respect to localization in different regions in space. In case of a quasi-free state this is true if its one-particle density matrix shows sufficiently fast decay (in position space). In order to overcome this restriction, highly occupied low momentum modes leading to long-range correlations have to be treated with a c-number substitution. I.e., coherent states on the bosonic Fock space are used to replace creation and annihilation operators of the low momentum modes by complex numbers. Since coherent states show an exact tensor product structure with respect to localization in different regions in space they fit seamlessly into the framework. Although there is no Bose–Einstein condensation in the two-dimensional Bose gas, we are also faced with highly occupied low momentum modes at very low temperatures. As explained in Remark 5 in Section 1.2 above, the use of coherent states for the low momentum modes naturally leads to the correct temperature dependence of the interaction energy in (2.1.1), whose origin is non-perturbative.

In order to be able to use a Fock space formalism, which is essential for the formalism of the c-number substitution, it will be necessary to replace the interaction potential v by an integrable potential $\tilde{v}$ with uniformly bounded Fourier transform. In contrast to the three-dimensional case, we will need that the integral of $\tilde{v}$ is suitably small in order to control various error terms. This replacement will be done in the first step of the proof.

We will frequently use the Heaviside step function in the proof and use the convention

$$\theta(x) = \begin{cases} 1 & \text{if } x \geq 0, \\ 0 & \text{if } x < 0. \end{cases} \tag{2.2.1}$$

Note in particular that $\theta(0) = 1$.

2.3 Reduction to integrable potentials with finite range

The statement of Theorem 2 is general in the sense that it allows interaction potentials that are infinitely ranged and possibly have infinite integral (e.g., in the case of a hard disk potential), while still having finite scattering length. In the following it will be convenient to work with integrable potentials with finite range. The first condition is of importance because for the Fock space formalism we need to assume that the interaction potential has a bounded Fourier transform. Since we want to prove a lower bound we can replace the original potential by a smaller one. The scattering length of the new potential is smaller, however. The following two lemmas quantify the change of the scattering length if we do such a replacement. We start with a lemma that quantifies the change of the scattering length when the potential is replaced by one that is cut off at some finite radius R_0.

Lemma 2. *Let v be a nonnegative radial potential with finite scattering length a. We denote by v_{R_0} the potential with cutoff at $R_0 > 0$ (i.e., $v_{R_0}(r) = \theta(R_0 - r)v(r)$) and its scattering length by a_{R_0}. Then*

$$\frac{1}{\ln(R/a_{R_0})} \geq \left(\ln(R/a) + \frac{1}{4\pi}\int_{|x|>R_0} v(|x|)\ln^2(|x|/a_{R_0})\,\mathrm{d}x\right)^{-1} \tag{2.3.1}$$

for all $R > R_0$.

Proof. The claim is equivalent to the inequality

$$\ln(a_{R_0}/a) \geq -\frac{1}{4\pi}\int_{|x|\geq R_0} v(|x|)\ln^2(|x|/a_{R_0})\,\mathrm{d}x. \tag{2.3.2}$$

To show (2.3.2), we use the variational principle of the scattering length for the potential with cutoff at R_1, where R_1 is such that $R_0 < R_1 < R$. Denote $\phi_{v_{R_0}}$ the minimizer of the energy functional (1.2.12) with potential v_{R_0}. Then we have

$$\begin{aligned}\frac{2\pi}{\ln(R/a_{R_1})} &\leq \int_{B_R}\left(|\nabla\phi_{v_{R_0}}|^2 + \frac{v_{R_1}}{2}|\phi_{v_{R_0}}|^2\right) = \frac{2\pi}{\ln(R/a_{R_0})} + \pi\int_{R_0}^{R_1} v(r)|\phi_{v_{R_0}}(r)|^2 r\,\mathrm{d}r \\ &= \frac{2\pi}{\ln(R/a_{R_0})}\left(1 + \frac{1}{2\ln(R/a_{R_0})}\int_{R_0}^{R_1} v(r)\ln^2(r/a_{R_0})r\,\mathrm{d}r\right).\end{aligned} \tag{2.3.3}$$

This implies

$$-\ln a_{R_1} \geq \frac{\ln(R/a_{R_0})}{1 + \frac{1}{2\ln(R/a_{R_0})}\int_{R_0}^{R_1} v(r)\ln^2(r/a_{R_0})r\,\mathrm{d}r} - \ln R \tag{2.3.4}$$

and by taking the limit $R \to \infty$, we obtain

$$\ln(a_{R_0}/a_{R_1}) \geq -\frac{1}{2}\int_{R_0}^{R_1} v(r)\ln^2(r/a_{R_0})r\,\mathrm{d}r. \tag{2.3.5}$$

Now we can take the limit $R_1 \to \infty$ and obtain (2.3.2). This completes the proof. □

When we apply Lemma 2, the cutoff parameter R_0 has to be chosen such that $a_{R_0} > 0$, which is the case if $v_{R_0} \not\equiv 0$. We shall choose R such that $\ln(R/a) \sim |\ln a^2\rho| \gg 1$, hence the second term on the right side of (2.3.1) is indeed a small correction to the first term. The relative error term we obtain this way is proportional to

$$\frac{1}{|\ln a^2\rho|}\int_{|x|>R_0} v(|x|)\ln^2(|x|/a_{R_0})\,\mathrm{d}x, \tag{2.3.6}$$

which is much smaller than other error terms we shall obtain below, see (2.18.16).

From now on we can thus assume that the interaction potential v has a fixed finite range R_0. For simplicity of notation, we shall drop the subscript R_0 from v and a.

The next lemma quantifies the change of the scattering length if we replace the potential v with finite range R_0 by a smaller potential $\tilde{v}$ whose integral is bounded by some number $4\pi\varphi > 0$. The error term we obtain is small as long as φ is much greater than $1/\ln(R/a)$. In particular, φ can be chosen as a small parameter, which is different from the corresponding three-dimensional case.

Lemma 3. *Let v be a nonnegative radial potential with finite range R_0 and scattering length a. For any $0 < \delta < 1$ and any $\varphi > 0$, there exists a potential $\tilde{v}$ with $0 \leq \tilde{v} \leq v$ such that $\int_{\mathbb{R}^2} \tilde{v}(|x|)\,\mathrm{d}x \leq 4\pi\varphi$ and the scattering length $\tilde{a}$ of $\tilde{v}$ satisfies*

$$\frac{1}{\ln(R/\tilde{a})} \geq \frac{1}{\ln(R/a)}\left(1 - \frac{1}{\sqrt{\varphi \ln(R/a)}} + \frac{\ln(1-\delta)}{\ln(R/a)}\right) \tag{2.3.7}$$

for all $R > R_0$.

Proof. Let

$$t = \inf\left\{s : \int_s^\infty rv(r)\,\mathrm{d}r < \infty\right\}. \tag{2.3.8}$$

and note that $t \leq a$ holds. To see this let $s > a$ and bound

$$\begin{aligned}\int_s^\infty rv(r)\,\mathrm{d}r &\leq \frac{1}{\ln^2(s/a)}\int_s^\infty rv(r)\ln^2(r/a)\,\mathrm{d}r \\ &\leq \frac{1}{\ln^2(s/a)}\int_a^\infty rv(r)\ln^2(r/a)\,\mathrm{d}r \leq \frac{4\pi\ln(R_0/a)}{\ln^2(s/a)},\end{aligned} \tag{2.3.9}$$

where the last inequality follows from an easy calculation, compare with [38, Eqs. (34)–(36)]. From this calculation we see that $\int_s^\infty rv(r)\,\mathrm{d}r$ is finite for all s with $s > a$.

Now we distinguish two cases. Assume first that $\int_t^\infty rv(r)\,\mathrm{d}r \geq 2\varphi$ (which includes the possibility that $v \to \infty$ in a non-integrable sense as $r \to t$). Then we choose $s \geq t$ such that $\int_s^\infty rv(r)\,\mathrm{d}r = 2\varphi$ and define $\tilde{v}(r) = v(r)\theta(r-s)$. Denote ϕ_v the solution to the zero-energy scattering equation $(-\Delta + \frac{v}{2})\phi_v = 0$ (or equivalently the minimizer of the energy functional (1.2.12)) on $B_R = \{x \in \mathbb{R}^2 : |x| \leq R\}$ with boundary condition $\phi_v|_{|x|=R} = 1$. Define the function

$$\phi(r) = \left(\phi_{\tilde{v}}(r) - \phi_{\tilde{v}}(s)\frac{\ln(R/r)}{\ln(R/s)}\right)\theta(r-s), \tag{2.3.10}$$

which is non-negative and continuous. We use ϕ as test function in the variational principle for the scattering length and obtain the upper bound

$$\begin{aligned} \frac{2\pi}{\ln(R/a)} &\leq \int_{B_R} \left(|\nabla\phi|^2 + \frac{v}{2}|\phi|^2 \right) = \int_{B_R} \overline{\phi} \left(-\Delta + \frac{v}{2} \right) \phi + \int_{\partial B_R} \overline{\phi} \nabla\phi \cdot n \\ &= -\frac{\phi_{\tilde{v}}(s)}{2\ln(R/s)} \int_{B_R} \overline{\phi}(|x|) v(|x|) \ln(R/|x|) \theta(|x| - s)\, \mathrm{d}x + \int_{\partial B_R} \overline{\phi} \nabla\phi \cdot n, \end{aligned} \tag{2.3.11}$$

where we integrated by parts and used the zero-energy scattering equation for $\tilde{v}$ as well as the fact that the function $r \mapsto \ln(R/r)$ is harmonic away from zero. In the boundary integral, we denoted by n the outward facing unit normal vector of the disk (which is in this case just the unit vector pointing in the radial direction). We note that the first term on the right-hand side is negative and can be dropped for an upper bound. Since $R > R_0$, the boundary term can be explicitly computed as

$$\int_{\partial B_R} \overline{\phi} \nabla\phi \cdot n = \frac{2\pi}{\ln(R/\tilde{a})} + \frac{2\pi\phi_{\tilde{v}}(s)}{\ln(R/s)}. \tag{2.3.12}$$

Hence,

$$\frac{1}{\ln(R/a)} \leq \frac{1}{\ln(R/\tilde{a})} + \frac{\phi_{\tilde{v}}(s)}{\ln(R/s)}. \tag{2.3.13}$$

Using the fact that $\phi_{\tilde{v}}(s)$ is always greater or equal than the asymptotic solution given by $\ln(s/\tilde{a})/\ln(R/\tilde{a})$, we obtain

$$\frac{\phi_{\tilde{v}}(s)}{\ln(R/s)} \leq \frac{1}{\ln(R/\tilde{a})} \cdot \frac{1}{1/\phi_{\tilde{v}}(s) - 1}. \tag{2.3.14}$$

We get an upper bound on $\phi_{\tilde{v}}(s)$ via the monotonicity of $\phi_{\tilde{v}}(r)$:

$$\frac{1}{\ln(R/a)} \geq \frac{1}{\ln(R/\tilde{a})} \geq \frac{1}{2} \int_s^\infty r v(r) \phi_{\tilde{v}}(r)^2 \,\mathrm{d}r \geq \phi_{\tilde{v}}(s)^2 \varphi. \tag{2.3.15}$$

Therefore,

$$\phi_{\tilde{v}}(s) \leq \frac{1}{\sqrt{\varphi \ln(R/a)}}. \tag{2.3.16}$$

In conclusion, we have shown that

$$\frac{1}{\ln(R/\tilde{a})} \geq \frac{1}{\ln(R/a)} \left(1 - \frac{1}{\sqrt{\varphi \ln(R/a)}} \right), \tag{2.3.17}$$

which proves the statement (for $\delta = 0$) in the first case.

It remains to consider the second case: Assume $\int_t^\infty rv(r)\,\mathrm{d}r = 2\varphi - T$ for some $T > 0$. We may assume further that $t > 0$, since if $t = 0$ we can take $\tilde{v} = v$ and there is nothing to prove. By the definition of t, we have that for any $0 < \delta < 1$

$$\int_{(1-\delta)t}^{t} rv(r)\,\mathrm{d}r = \infty. \tag{2.3.18}$$

Therefore there exists a $\tau = \tau(T, \delta)$ such that

$$\int_{(1-\delta)t}^{t} r\min\{v(r), \tau\}\,\mathrm{d}r = T. \tag{2.3.19}$$

We define

$$\tilde{v}(r) = \begin{cases} v(r) & \text{if } r \geq t, \\ \min\{v(r), \tau\} & \text{if } (1-\delta)t \leq r < t, \\ 0 & \text{else.} \end{cases} \tag{2.3.20}$$

Note that

$$\int_0^\infty r\tilde{v}(r)\,\mathrm{d}r = \int_{(1-\delta)t}^\infty r\tilde{v}(r)\,\mathrm{d}r = 2\varphi. \tag{2.3.21}$$

By the same argument as before (cf. equation (2.3.13) with $s = t$) and with this definition of $\tilde{v}$, we obtain

$$\frac{1}{\ln(R/a)} \leq \frac{1}{\ln(R/\tilde{a})} + \frac{\phi_{\tilde{v}}(t)}{\ln(R/t)}. \tag{2.3.22}$$

Similarly to (2.3.15), we have

$$\frac{1}{\ln(R/a)} \geq \frac{1}{\ln(R/\tilde{a})} \geq \frac{1}{2}\int_{(1-\delta)t}^\infty r\tilde{v}(r)\phi_{\tilde{v}}(r)^2\,\mathrm{d}r \geq \phi_{\tilde{v}}((1-\delta)t)^2\varphi. \tag{2.3.23}$$

Therefore,

$$\phi_{\tilde{v}}((1-\delta)t) \leq \frac{1}{\sqrt{\varphi\ln(R/a)}}. \tag{2.3.24}$$

Using Gauss' theorem, we have

$$\int_{|x|\leq r} \Delta\phi_{\tilde{v}} = \int_{|x|=r} \nabla\phi_{\tilde{v}}\cdot n = 2\pi r\phi_{\tilde{v}}'(r). \tag{2.3.25}$$

Since the integrand on the left-hand side is nonnegative pointwise, we have that $r \mapsto r\phi_{\tilde{v}}'(r)$ is monotone increasing. This implies for any $s \leq r$ and for $r \geq R_0$

$$s\phi_{\tilde{v}}'(s) \leq r\phi_{\tilde{v}}'(r) = \frac{1}{\ln(R/\tilde{a})}. \tag{2.3.26}$$

Thus, using the fundamental theorem of calculus,

$$\begin{aligned}\phi_{\tilde v}(t)-\phi_{\tilde v}((1-\delta)t) &= \delta t\int_0^1 \phi'_{\tilde v}((1-\delta w)t)\,\mathrm{d}w\\ &\leq \frac{\delta}{\ln(R/\tilde a)}\int_0^1 \frac{\mathrm{d}w}{1-\delta w} = -\frac{\ln(1-\delta)}{\ln(R/\tilde a)}.\end{aligned} \tag{2.3.27}$$

Putting (2.3.22), (2.3.24) and (2.3.27) together as well as using $t \leq a$ and $\tilde a \leq a$, we obtain

$$\begin{aligned}\frac{1}{\ln(R/a)} &\leq \frac{1}{\ln(R/\tilde a)} + \frac{\phi_{\tilde v}(t)}{\ln(R/t)}\\ &\leq \frac{1}{\ln(R/\tilde a)} + \frac{1}{\ln(R/t)}\left(\phi_{\tilde v}(t)-\phi_{\tilde v}((1-\delta)t)\right) + \frac{1}{\ln(R/t)}\frac{1}{\sqrt{\varphi\ln(R/a)}}\\ &\leq \frac{1}{\ln(R/\tilde a)} - \frac{\ln(1-\delta)}{\ln(R/a)^2} + \frac{1}{\ln(R/a)}\frac{1}{\sqrt{\varphi\ln(R/a)}}.\end{aligned} \tag{2.3.28}$$

Rearranging the terms, we obtain (2.3.7). □

In the following we denote by $\tilde v$ the interaction potential that is obtained from v (which is assumed to have finite range R_0 as discussed after Lemma 2) by cutting it as indicated by Lemma 3, such that its integral is bounded by $4\pi\varphi > 0$. As mentioned already before we have $H_N \geq \tilde H_N$, where $\tilde H_N$ denotes the Hamiltonian with v replaced by $\tilde v$.

2.4 Fock space

In our proof we relax the restriction on the number of particles, which is possible for a lower bound and is motivated by the fact that this allows us to use the formalism of c-number substitution, as detailed in the next section. We denote by $\mathcal{F}$ the bosonic Fock space and define the Fock space Hamiltonian

$$\mathbb{H} = \mathbb{T} + \mathbb{V} + \mathbb{K} + \mu_0 N \tag{2.4.1}$$

with

$$\mathbb{T} = \sum_p \left(p^2-\mu_0\right) a_p^\dagger a_p, \quad \mathbb{V} = \frac{1}{2|\Lambda|}\sum_{p,k,\ell} \hat v(p) a_{k+p}^\dagger a_{\ell-p}^\dagger a_k a_\ell \tag{2.4.2}$$

and

$$\mathbb{K} = \frac{4\pi C}{|\Lambda||\ln a^2\rho|}\left(\mathbb{N}-N\right)^2. \tag{2.4.3}$$

Here, the chemical potential μ_0 is given by (1.2.7) and $a_p^\dagger$ and a_p are the usual creation and annihilation operators on Fock space that create or annihilate a plane wave with momentum p, respectively. The sums over p, k and ℓ are taken over $\frac{2\pi}{L}\mathbb{Z}^2$. By $\hat{v}$ we denote the Fourier transform of $\tilde{v}$ (we drop the ~ in the Fourier transform for notational clarity), which is given by $\hat{v}(p) = \int_\Lambda \tilde{v}(d(x,0))\, \mathrm{e}^{-ipx}\, \mathrm{d}x = \int_{\mathbb{R}^2} \tilde{v}(|x|)\, \mathrm{e}^{-ipx}\, \mathrm{d}x$. Here and in the following we assume that $L > 2R_0$, which is no restriction since we are interested in the thermodynamic limit $L \to \infty$. Note that $\hat{v}$ is uniformly bounded, which is one reason we introduced $\tilde{v}$: We have

$$|\hat{v}(p)| \leq \hat{v}(0) \leq 4\pi\varphi. \tag{2.4.4}$$

The number operator is defined by

$$\mathbb{N} = \sum_p a_p^\dagger a_p \tag{2.4.5}$$

and the operator $\mathbb{K}$ was introduced in order to control the number of particles in the system after the extension to Fock space.

Recall that we defined the total Hamiltonian for N particles by H_N (in Eq. (1.2.1)) and that we denote by $\tilde{H}_N$ the operator H_N where v is replaced by $\tilde{v}$. We then have $H_N \geq \tilde{H}_N = \mathbb{H}P_N$, where P_N is the projection on the Fock space sector with N particles. This implies in particular that

$$\mathrm{Tr}_{\mathcal{H}_N} \exp(-\beta H_N) \leq \mathrm{Tr}_{\mathcal{H}_N} \exp(-\beta \tilde{H}_N) \leq \mathrm{Tr}_{\mathcal{F}} \exp(-\beta \mathbb{H}). \tag{2.4.6}$$

We will proceed deriving an upper bound for the expression on the right-hand side.

2.5 Coherent states

We use the method of coherent states (see, e.g., [48]) in order to obtain an upper bound on the partition function $\mathrm{Tr}_{\mathcal{F}} \exp(-\beta\mathbb{H})$. This method is based on the fact that coherent states are eigenfunctions of the annihilation operators, which can be used to replace the operators a_p and $a_p^\dagger$ by complex numbers. This procedure is also called c-number substitution. Although we have no condensate in our system, this separate treatment of a certain number of low momentum modes is necessary for low temperatures, as pointed out in the proof strategy in Section 2.2. We start by introducing the necessary notation related to the c-number substitution.

Pick some $p_c \geq 0$ and write $\mathcal{F} = \mathcal{F}_< \otimes F_>$. Here $\mathcal{F}_<$ and $\mathcal{F}_>$ denote the Fock spaces corresponding to the modes $|p| < p_c$ and $|p| \geq p_c$, respectively. We define $M = \sum_{|p|<p_c} 1 =$

$\#\{p \in \frac{2\pi}{L}\mathbb{Z}^2 : |p| < p_c\}$ and introduce for $z \in \mathbb{C}^M$ the coherent state $|z\rangle \in \mathcal{F}_<$ by

$$|z\rangle = \exp\left(\sum_{|p|<p_c} z_p a_p^\dagger - \bar{z}_p a_p\right)\Pi_0 =: U(z)\Pi_0. \tag{2.5.1}$$

Here Π_0 is the vacuum state in $\mathcal{F}_<$ and last equality defines the Weyl operator $U(z)$. The lower symbol $\mathbb{H}_s(z)$ of $\mathbb{H}$ is the operator on $\mathcal{F}_>$ given by the partial inner product

$$\mathbb{H}_s(z) = \langle z|\mathbb{H}|z\rangle\,. \tag{2.5.2}$$

We can use the fact that $a_p\,|z\rangle = z_p\,|z\rangle$ and obtain the lower symbol by simply replacing all a_p by z_p and $a_p^\dagger$ by $\bar{z}_p$ for $|p| < p_c$. The upper symbol of an operator is the operator-valued function that is obtained by starting from the anti-normal ordered form of the operator and then replacing a_p by z_p and $a_p^\dagger$ by $\bar{z}_p$ for $|p| < p_c$. This implies that the upper symbol can be calculated from the lower symbol by replacing for example $|z_p|^2$ by $|z_p|^2 - 1$ and similarly for other polynomials in z_p (see [48] for more details). The upper symbol $\mathbb{H}^s(z)$ of $\mathbb{H}$ satisfies

$$\mathbb{H} = \int_{\mathbb{C}^M} \mathbb{H}^s(z)|z\rangle\langle z|\,\mathrm{d}z, \tag{2.5.3}$$

where $\mathrm{d}z = \prod_{i=1}^M \frac{\mathrm{d}z_i}{\pi}$, $\mathrm{d}z_i = \mathrm{d}x_i\,\mathrm{d}y_i$ is the product measure of the real and imaginary part of $z_i \in \mathbb{C}$. The Berezin–Lieb inequality [4, 5, 44, 48] implies

$$\mathrm{Tr}_{\mathcal{F}} \exp(-\beta\mathbb{H}) \le \int_{\mathbb{C}^M} \mathrm{Tr}_{\mathcal{F}} \exp(-\beta\mathbb{H}^s(z))\,\mathrm{d}z. \tag{2.5.4}$$

We prefer to work with the lower symbol instead, and therefore will replace the upper by the lower symbol on the right-hand side of (2.5.4). Let $\Delta\mathbb{H}(z) = \mathbb{H}_s(z) - \mathbb{H}^s(z)$ be the difference between the two symbols, which reads

$$\begin{aligned}\Delta\mathbb{H}(z) = &\sum_{|p|<p_c}\left(p^2 - \mu_0\right) + \frac{1}{2|\Lambda|}\Big[\hat{v}(0)\left(2M\mathbb{N}_s(z) - M^2\right) \\ &+ 2\sum_{|\ell|<p_c,|k|\ge p_c} \hat{v}(\ell-k)a_k^\dagger a_k + \sum_{|\ell|,|k|<p_c} \hat{v}(\ell-k)\left(2|z_k|^2 - 1\right)\Big] \\ &+ \frac{4\pi C}{|\Lambda||\ln a^2\rho|}\left[2|z|^2 + M\left(2\mathbb{N}_s(z) - 2N - M\right)\right].\end{aligned} \tag{2.5.5}$$

We therefore have (using the uniform bound $|\hat{v}(p)| \le \hat{v}(0) \le 4\pi\varphi$)

$$\Delta\mathbb{H}(z) \le M\left(p_c^2 - \mu_0\right) + \frac{8\pi\varphi}{|\Lambda|}M\mathbb{N}_s(z) + \frac{8\pi C}{|\Lambda||\ln a^2\rho|}\left[|z|^2 + M\left(\mathbb{N}_s(z) - N\right)\right]. \tag{2.5.6}$$

The lower symbol of $\mathbb{K}$ reads

$$\mathbb{K}_s(z) = \frac{4\pi C}{|\Lambda||\ln a^2\rho|}\left((\mathbb{N}_s(z) - N)^2 + |z|^2\right) \geq \frac{4\pi C}{|\Lambda||\ln a^2\rho|}(\mathbb{N}_s(z) - N)^2 \tag{2.5.7}$$

and allows us to estimate

$$\begin{aligned}\tfrac{1}{2}\mathbb{K}_s(z) - \Delta\mathbb{H}(z) \geq & -M(p_c^2 - \mu_0) - \frac{8\pi N}{|\Lambda|}\left(\varphi M + \frac{C}{|\ln a^2\rho|}\right) \\ & - \frac{32\pi C(M+1)^2}{|\Lambda||\ln a^2\rho|}\left(1 + \frac{\varphi|\ln a^2\rho|}{C}\right)^2 \\ =: & -Z^{(1)}.\end{aligned} \tag{2.5.8}$$

Note that $M \sim p_c^2|\Lambda|$ in the thermodynamic limit. We will choose the parameters p_c, φ and C such that $Z^{(1)} \ll |\Lambda|\rho^2/|\ln a^2\rho|$ for small $a^2\rho$. We also define

$$F_z(\beta) = -\frac{1}{\beta}\ln \mathrm{Tr}_{\mathcal{F}_>} \exp\left(-\beta\left(\mathbb{T}_s(z) + \mathbb{V}_s(z) + \tfrac{1}{2}\mathbb{K}_s(z)\right)\right). \tag{2.5.9}$$

Eq. (2.5.4) and the above estimates imply the bound

$$-\frac{1}{\beta}\ln \mathrm{Tr}_{\mathcal{F}} \exp(-\beta\mathbb{H}) \geq \mu_0 N - \frac{1}{\beta}\ln\int_{\mathbb{C}^M} \exp(-\beta F_z(\beta))\,\mathrm{d}z - Z^{(1)}. \tag{2.5.10}$$

In the following subsections we will derive a lower bound on $F_z(\beta)$.

The free energy $F_z(\beta)$ can also be written in terms of the free energy of a Gibbs state. In fact, let Γ^z be the Gibbs state of $\mathbb{T}_s(z) + \mathbb{V}_s(z) + \frac{1}{2}\mathbb{K}_s(z)$ on $\mathcal{F}_>$, i.e.,

$$\Gamma^z = \frac{\exp\left(-\beta\left[\mathbb{T}_s(z) + \mathbb{V}_s(z) + \frac{1}{2}\mathbb{K}_s(z)\right]\right)}{\mathrm{Tr}_{\mathcal{F}_>}\exp\left(-\beta\left[\mathbb{T}_s(z) + \mathbb{V}_s(z) + \frac{1}{2}\mathbb{K}_s(z)\right]\right)} \tag{2.5.11}$$

and define

$$\Upsilon^z = U(z)\Pi_0 U(z)^\dagger \otimes \Gamma^z \tag{2.5.12}$$

on $\mathcal{F}$. With these definitions we obtain the identity

$$F_z(\beta) = \mathrm{Tr}_{\mathcal{F}}\left[\left(\mathbb{T} + \mathbb{V} + \tfrac{1}{2}\mathbb{K}\right)\Upsilon^z\right] - \frac{1}{\beta}S(\Upsilon^z), \tag{2.5.13}$$

where $S(\Upsilon^z) = -\mathrm{Tr}_{\mathcal{F}}[\Upsilon^z \ln \Upsilon^z]$ is the von Neumann entropy of the state Υ^z (which equals the one of Γ^z).

2.6 Relative entropy and a priori bounds

To prove a lower bound on $F_z(\beta)$ we will need some information on the state Υ^z defined in (2.5.12) above. The a priori information that is being used is a bound on the relative entropy (to be defined below) of Υ^z with respect to a suitable reference state describing non-interacting bosons and a bound on the expected number of particles in the system. To obtain this a priori information we will assume that a certain upper bound on $F_z(\beta)$ holds. This does not lead to a loss of generality because there will be nothing to prove if the assumption is not fulfilled. That is, the statement will hold independently of the assumptions.

Let Γ_0 be the Gibbs state on $\mathcal{F}_>$ for the kinetic energy operator $\mathbb{T}_s(z)$ (which is independent of z) and define the state Ω_0^z on $\mathcal{F}$ by $\Omega_0^z = U(z)\Pi_0 U(z)^\dagger \otimes \Gamma_0$. Since $\mathbb{V} \geq 0$ we have

$$F_z(\beta) \geq -\frac{1}{\beta}\ln\left(\mathrm{Tr}_{\mathcal{F}_>}\left[\mathrm{e}^{-\beta\mathbb{T}_s(z)}\right]\right) + \frac{1}{2}\,\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{K}\Upsilon^z\right] + \frac{1}{\beta}S\left(\Upsilon^z, \Omega_0^z\right), \tag{2.6.1}$$

where

$$S\left(\Upsilon^z, \Omega_0^z\right) = \mathrm{Tr}_{\mathcal{F}}\left[\Upsilon^z\left(\ln\Upsilon^z - \ln\Omega_0^z\right)\right] \tag{2.6.2}$$

denotes the relative entropy of Υ^z with respect to Ω_0^z. Since Υ^z and Ω_0^z are equal on $\mathcal{F}_<$ we have $S\left(\Upsilon^z, \Omega_0^z\right) = S\left(\Gamma^z, \Gamma_0\right)$. We distinguish two cases: Either

$$F_z(\beta) \geq -\frac{1}{\beta}\ln\left(\mathrm{Tr}_{\mathcal{F}_>}\left[\mathrm{e}^{-\beta\mathbb{T}_s(z)}\right]\right) + \frac{8\pi|\Lambda|\rho^2}{|\ln a^2\rho|} \tag{2.6.3}$$

holds or it does not hold. In the latter case we have

$$S\left(\Upsilon^z, \Omega_0^z\right) = S\left(\Gamma^z, \Gamma_0\right) \leq \frac{8\pi|\Lambda|\beta\rho^2}{|\ln a^2\rho|} \tag{2.6.4}$$

as well as

$$\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{K}\Upsilon^z\right] \leq \frac{16\pi|\Lambda|\rho^2}{|\ln a^2\rho|}. \tag{2.6.5}$$

From now on we will assume to be in the second case. The lower bound we are going to derive on $F_z(\beta)$ will actually be worse than (2.6.3) above, that is, the bound is true in any case, irrespective of whether the assumptions (2.6.4) and (2.6.5) hold.

Eq. (2.6.5) implies the following upper bound on $|z|^2$:

$$\begin{aligned} |z|^2 - N &\leq \mathrm{Tr}_{\mathcal{F}}\left[(\mathbb{N}-N)\,\Upsilon^z\right] \leq \left(\mathrm{Tr}_{\mathcal{F}}\left[(\mathbb{N}-N)^2\,\Upsilon^z\right]\right)^{1/2} \\ &= \left(\frac{|\Lambda||\ln a^2\rho|}{4\pi C}\right)^{1/2}\left(\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{K}\Upsilon^z\right]\right)^{1/2} \leq \frac{2}{\sqrt{C}}|\Lambda|\rho. \end{aligned} \tag{2.6.6}$$

In other words,

$$\rho_z := \frac{|z|^2}{|\Lambda|} \leq \rho\left(1 + \frac{2}{\sqrt{C}}\right). \tag{2.6.7}$$

We will choose $C \gg 1$ below.

2.7 Replacing vacuum

In this section, we replace the vacuum state Π_0 in the definition of Υ^z in (2.5.12) by a more general quasi-free state Π on $\mathcal{F}_<$ and estimate the effect of this replacement on (2.5.13). The replacement will become relevant in Section 2.15 when we estimate the relative entropy of the above state with respect to a certain quasi-free state describing non-interacting bosons. For that purpose we require the momentum distribution to be sufficiently smooth and do not want it to jump to zero for momenta less than p_c.

Let Π be the unique quasi-free state on $\mathcal{F}_<$ whose one-particle density matrix is given by

$$\pi = \sum_{|p|<p_c} \pi_p |p\rangle\langle p|. \tag{2.7.1}$$

The coefficients π_p will be chosen later. We denote the trace of π by P. Define the state Υ^z_π on $\mathcal{F}$ by

$$\Upsilon^z_\pi = U(z)\Pi U(z)^\dagger \otimes \Gamma^z. \tag{2.7.2}$$

Using $|\hat{v}(p)| \leq 4\pi\varphi$, we see that

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{V}\left(\Upsilon^z_\pi - \Upsilon^z\right)\right] &= \frac{1}{2|\Lambda|}\hat{v}(0)\left(P^2 + 2P\,\mathrm{Tr}_{\mathcal{F}_>}\left[\mathbb{N}_s(z)\Gamma^z\right]\right) \\ &\quad + \frac{1}{2|\Lambda|}\sum_{|k|,|\ell|<p_c} \hat{v}(k-\ell)\left[\pi_k\pi_\ell + 2|z_k|^2\pi_\ell\right] \\ &\quad + \frac{1}{|\Lambda|}\sum_{|k|<p_c,|\ell|\geq p_c} \hat{v}(k-\ell)\pi_k\,\mathrm{Tr}_{\mathcal{F}_>}\left[a^\dagger_\ell a_\ell \Gamma^z\right] \\ &\leq \frac{4\pi\varphi}{|\Lambda|}\left(P^2 + 2P\,\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\Upsilon^z\right]\right). \end{aligned} \tag{2.7.3}$$

To obtain the first equality[1] we split the sum over p into two terms, one with $p = 0$ and the

[1] We note that in [70, first line of (2.5.4)] there is an erroneous term $-2\sum_{|k|<p_c}\pi_k|z_k|^2$. Since it is negative it was dropped for the following estimate, which resulted in an analogous upper bound on $\mathrm{Tr}_{\mathcal{F}}[\mathbb{V}(\Upsilon^z_\pi - \Upsilon^z)]$.

other one with $p \neq 0$. The $p = 0$ contribution is given by

$$\begin{aligned}&\frac{1}{2|\Lambda|}\sum_{k,\ell}\hat{v}(0)\operatorname{Tr}_{\mathcal{F}}\left[a_k^\dagger a_\ell^\dagger a_k a_\ell \left(U(z)(\Pi-\Pi_0)U(z)^\dagger\otimes\Gamma^z\right)\right]\\&\quad=\frac{\hat{v}(0)}{2|\Lambda|}\left(P^2+2P\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}_{\mathrm{s}}(z)\Gamma^z]+\sum_{|k|<p_{\mathrm{c}}}(\pi_k^2+2\pi_k|z_k|^2)\right).\end{aligned} \tag{2.7.4}$$

The $p \neq 0$ contribution on the other hand is given by

$$\begin{aligned}&\frac{1}{2|\Lambda|}\sum_{\substack{k,\ell\\p\neq 0}}\hat{v}(p)\operatorname{Tr}_{\mathcal{F}}\left[a_{k+p}^\dagger a_{\ell-p}^\dagger a_k a_\ell\left(U(z)(\Pi-\Pi_0)U(z)^\dagger\otimes\Gamma^z\right)\right] \qquad (2.7.5)\\&=\frac{1}{2|\Lambda|}\sum_{\substack{|k|,|\ell|<p_{\mathrm{c}}\\k\neq\ell}}\hat{v}(\ell-k)(\pi_\ell\pi_k+2\pi_\ell|z_k|^2)+\frac{1}{|\Lambda|}\sum_{\substack{|\ell|<p_{\mathrm{c}}\\|k|\geq p_{\mathrm{c}}}}\hat{v}(\ell-k)\pi_\ell\operatorname{Tr}_{\mathcal{F}_>}\left[a_k^\dagger a_k\Gamma^z\right].\end{aligned}$$

If we now put back the $k = \ell$ term into the first sum of the right side of (2.7.5) we have to subtract exactly the last sum of the right side of (2.7.4) and arrive thus at the first equality of (2.7.3). In (2.6.6) we have shown that $\operatorname{Tr}_{\mathcal{F}}[\mathbb{N}\Upsilon^z] \leq N(1+2/\sqrt{C})$ and we therefore obtain from (2.7.3)

$$\operatorname{Tr}_{\mathcal{F}}[\mathbb{V}\Upsilon^z] \geq \operatorname{Tr}_{\mathcal{F}}[\mathbb{V}\Upsilon^z_\pi] - Z^{(2)} \tag{2.7.6}$$

with

$$Z^{(2)} := \frac{4\pi\varphi P^2}{|\Lambda|} + \frac{8\pi P\varphi}{|\Lambda|}N\left(1+\frac{2}{\sqrt{C}}\right). \tag{2.7.7}$$

We will choose $\varphi \gg |\ln a^2\rho|^{-1}$ and $C \gg 1$. Hence, $Z^{(2)} \ll |\Lambda|\rho^2/|\ln a^2\rho|$ as long as $\varphi P \ll N/|\ln a^2\rho|$.

The replacement of Υ^z by Υ^z_π causes also a change in the kinetic energy that is given by

$$\operatorname{Tr}_{\mathcal{F}}[\mathbb{T}\Upsilon^z] = \operatorname{Tr}_{\mathcal{F}}[\mathbb{T}\Upsilon^z_\pi] - \sum_{|p|<p_{\mathrm{c}}}\left(p^2-\mu_0\right)\pi_p. \tag{2.7.8}$$

By combining (2.5.13), (2.7.6) and (2.7.8) we therefore obtain the lower bound

$$F_z(\beta) \geq \operatorname{Tr}_{\mathcal{F}}[(\mathbb{T}+\mathbb{V})\Upsilon^z_\pi] + \frac{1}{2}\operatorname{Tr}_{\mathcal{F}}[\mathbb{K}\Upsilon^z] - \frac{1}{\beta}S(\Upsilon^z) - \sum_{|p|<p_{\mathrm{c}}}\left(p^2-\mu_0\right)\pi_p - Z^{(2)}. \tag{2.7.9}$$

2.8 Dyson Lemma

As already mentioned in the proof strategy in Section 2.2, in order to be in a perturbative regime we have to replace the short ranged and possibly very strong interaction potential $\tilde{v}$ by a softer interaction potential with longer range. To achieve this goal we have to pay with a certain amount of kinetic energy. More precisely, we will only use modes with momenta much larger than $\beta^{-1/2}$ for this proecedure because the other momentum modes are needed to obtain the free energy $f_0(\beta, \rho)$ of the ideal gas.

To separate the high momentum part of the kinetic energy (which is the relevant part contributing to the interaction energy) from the low momentum part, we choose a radial cutoff function $\chi : \mathbb{R}^2 \to [0, 1]$ and define

$$h(x) = \frac{1}{|\Lambda|} \sum_p (1 - \chi(p)) \, \mathrm{e}^{-ipx} \,. \tag{2.8.1}$$

We assume that $\chi(p) \to 1$ sufficiently fast as $|p| \to \infty$ so that $h \in L^1(\Lambda) \cap L^\infty(\Lambda)$. Define further for $R_0 < R < L/2$

$$f_R(x) = \sup_{|y| \leq R} |h(x - y) - h(x)| \quad \text{and} \quad w_R(x) = \frac{2}{\pi} f_R(x) \int_\Lambda f_R(y) \, \mathrm{d}y. \tag{2.8.2}$$

Finally, we introduce the soft potential U_R which is a nonnegative function supported on the interval $[R_0, R]$. Its integral should satisfy

$$\int_{R_0}^R U_R(t) \ln(t/\tilde{a}) t \, \mathrm{d}t \leq 1. \tag{2.8.3}$$

We then have the following statement.

Lemma 4. *Let $y_1, \ldots, y_n$ be n points in Λ and denote by $y_{\mathrm{NN}}(x)$ the nearest neighbor of $x \in \Lambda$ among the points y_i. Then for any $\epsilon > 0$, we have*

$$-\nabla \chi(p)^2 \nabla + \frac{1}{2} \sum_{i=1}^n \tilde{v}(d(x, y_i)) \geq (1 - \epsilon) U_R(d(x, y_{\mathrm{NN}}(x))) - \frac{1}{\epsilon} \int_{\mathbb{R}_+} U_R(t) t \, \mathrm{d}t \sum_{i=1}^n w_R(x - y_i). \tag{2.8.4}$$

We remark that $y_{\mathrm{NN}}(x)$ is well defined except on a set of zero measure. The Lemma above is a two-dimensional version of [70, Lemma 2]. It is referred to as Dyson Lemma because Dyson was the first to prove a statement of this kind in his treatment of the dilute Bose gas at $T = 0$ in [23]. A version of the Dyson Lemma for two and three space dimensions, where only the high momentum modes are used to replace the interaction potential by a softer one, appeared for the first time in [45]. The proof of Lemma 4 can be obtained by combining the ideas of the proofs of [70, Lemma 2] and [45, Lemma 7]. The main differences between Lemma 4 and [45, Lemma 7] are the boundary conditions for the Laplacian and the fact that we do not assume a minimal distance between the particles here. Since the proof of [45, Lemma 7] was not spelled out in detail, we include a proof of Lemma 4 in Appendix 2.A.

We will use Lemma 4 for a lower bound on the operator $\mathbb{T} + \mathbb{V}$. In the Fock space sector with n particles this operator reads

$$\tilde{H}_n = \sum_{j=1}^{n} \Bigg[-\Delta_j + \frac{1}{2} \sum_{\substack{i \\ i \neq j}} \tilde{v}(d(x_i, x_j)) \Bigg]. \tag{2.8.5}$$

We want to keep a small part of the total kinetic energy for later use and therefore write for $0 < \kappa < 1$

$$p^2 = p^2 \left(1 - (1 - \kappa)\chi(p)^2\right) + (1 - \kappa) p^2 \chi(p)^2. \tag{2.8.6}$$

The kinetic term in $\tilde{H}_n$ will be split accordingly and we apply Lemma 4 to the last part of the kinetic term plus the potential term. Using also the positivity of $\tilde{v}$, we obtain for any subset $J_j \subset \{1, \dots j-1, j+1, \dots, n\}$

$$\begin{aligned} -\Delta_j + \frac{1}{2} \sum_{i \neq j} \tilde{v}(d(x_i, x_j)) \geq{}& -\nabla_j (1 - (1 - \kappa)\chi(p_j)^2) \nabla_j \\ &+ (1 - \epsilon)(1 - \kappa) U_R \left(d \left(x_j, x_{\mathrm{NN}}^{J_j}(x_j) \right) \right) - \frac{1}{\epsilon} \int_{\mathbb{R}_+} U_R(t) t \, \mathrm{d}t \sum_{i \in J_j} w_R(x_j - x_i). \end{aligned} \tag{2.8.7}$$

Here $x_{\mathrm{NN}}^{J_j}(x_j)$ denotes the nearest neighbor of x_j among the points x_i whose index i is contained in J_j, and interaction terms for particles $k \notin J_j$ are simply dropped for a lower bound. The subset J_j is defined via the following construction (which is not unique). Fix x_j and consider those x_i whose distance to the nearest neighbor (among all other x_k, $k \neq i, j$) is at least $R/5$, and add the corresponding index i to the set. Next, we go in some order through the set $\{x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n\}$ and add i to the set if $d(x_i, x_k) \geq R/5$ for all k that are already in the set J_j. Note that this last step depends on the ordering of the x_i and therefore J_j will depend on the ordering as well. Hence, the right side of (2.8.7) is not permutation symmetric and strictly speaking it should be replaced by its symmetrization. We do not need to do this, however, as we are only interested in expectation values of this potential in bosonic (permutation symmetric) states anyway.

The motivation to introduce J_j is the following. By definition, all particles whose index is contained in J_j have a minimum distance $R/5$ to their nearest neighbor, which is needed in order to control the error terms coming from w_R. On the other hand, the set J_j is constructed to be maximal in the sense that if $l \notin J_j$, then there exists a particle x_k with $k \in J_j$ such that $d(x_l, x_k) < R/5$. In other words, we need the disks of radius R centered at the particle coordinates to be able to have sufficient overlap in order to obtain the desired lower bound. For certain values of z the system could be far from homogeneous[2] and many particles could cluster in a relatively small volume; we want to be able to detect this as an increase in the interaction energy.

2.9 Filling the holes

After having applied Lemma 4 we want to replace the resulting interaction potential U_R by a potential without a hole of radius R_0 at the origin because it will be advantageous to work with a potential of positive type. To obtain such a potential we use Lemma 5 below. Its proof requires a different technique than the corresponding Lemma in the three-dimensional case [70, Lemma 3], due to the fact that a sufficiently weak attractive potential in three dimensions has no bound state, while it always does in one or two dimensions.

For some unit vector $e \in \mathbb{R}^2$ we define the function $j : \mathbb{R}_+ \to \mathbb{R}_+$ by

$$j(t) = \frac{32}{\pi} \int_{\mathbb{R}^2} \theta\left(\frac{1}{2} - |y|\right) \theta\left(\frac{1}{2} - |y - te|\right) \mathrm{d}y. \tag{2.9.1}$$

Note that the support of the function j is given by the interval $[0, 1]$ and that we have $\int_0^1 j(t)t \,\mathrm{d}t = 1$. An explicit computation yields

$$j(t) = \frac{16}{\pi} \left[\arccos(t) - t\sqrt{1 - t^2}\right] \mathbb{1}_{[0,1]}(t), \tag{2.9.2}$$

where $\mathbb{1}_{[0,1]}$ denotes the characteristic function of the interval $[0, 1]$. The potential we intend to work with is $\tilde{U}_R(t) = R^{-2} \ln(R/\tilde{a})^{-1} j(t/R)$. To obtain this potential we choose $U_R(t) = \tilde{U}_R(t)\theta(t - R_0)$ when we apply the Dyson Lemma. This choice indeed satisfies the integral condition (2.8.3), since

$$\begin{aligned} \int_{R_0}^{R} U_R(t) \ln(t/\tilde{a}) t \,\mathrm{d}t &= \frac{1}{R^2 \ln(R/\tilde{a})} \int_{R_0}^{R} j(t/R) \ln(t/\tilde{a}) t \,\mathrm{d}t \\ &\leq \frac{1}{R^2} \int_{R_0}^{R} j(t/R) t \,\mathrm{d}t = \int_{R_0/R}^{1} j(t) t \,\mathrm{d}t \leq \int_0^1 j(t) t \,\mathrm{d}t = 1. \end{aligned} \tag{2.9.3}$$

[2]Recall that $z = (z_1, \ldots, z_M) \in \mathbb{C}^M$ is the complex vector introduced in Section 2.5.

The following lemma will allow us to quantify the error we make when we replace U_R by $\tilde{U}_R$.

Lemma 5. *Let $y_1, \dots, y_n$ denote n points in Λ, with $d(y_i, y_j) \geq R/5$ for $i \neq j$ and let $R_0 < R/10$. Then*

$$-\Delta - \frac{1}{R_0^2 \ln(R/R_0)} \sum_{i=1}^{n} \theta(R_0 - d(x, y_i)) \geq -\frac{\tilde{C}}{R^2} \sum_{i=1}^{n} \theta(R/10 - d(x, y_i)) \tag{2.9.4}$$

holds for a universal constant $\tilde{C} > 0$.

Proof. It is sufficient to prove that

$$\begin{aligned} &\int_{|x| \leq R/10} \left(|\nabla \phi(x)|^2 - \frac{1}{R_0^2 \ln(R/R_0)} \theta(R_0 - |x|) |\phi(x)|^2 \right) \mathrm{d}x \\ &\qquad \geq -\frac{\tilde{C}}{R^2} \int_{|x| \leq R/10} |\phi(x)|^2 \, \mathrm{d}x \end{aligned} \tag{2.9.5}$$

holds for any function $\phi \in H^1(\mathbb{R}^2)$ with $\tilde{C} > 0$ being independent of that function. In other words, we need to show that the lowest eigenvalue of the quadratic form on the left-hand side of Eq. (2.9.5) is bounded from below by a constant times $-R^{-2}$.

Denote by E_R^{N} this lowest eigenvalue and by ϕ_R^{N} the corresponding normalized eigenfunction. We will bound E_R^{N} from below in terms of E_0, the lowest eigenvalue of the Schrödinger operator

$$h = -\Delta - \frac{1}{R_0^2 \ln(R/R_0)} \theta(R_0 - |x|) \tag{2.9.6}$$

acting on $L^2(\mathbb{R}^2)$. By rearrangement ϕ_R^{N} is a radial decreasing function, satisfying Neumann boundary conditions. Choose $\lambda \in C^\infty([0, \infty))$ such that $\lambda(0) = 1$, $\lambda'(0) = 0$, $\lambda(t) = 0$ for $t \geq 1$ and $|\lambda'(t)|^2 \leq 2$, $|\lambda(t)| \leq 1$ for all $t \geq 0$. We define

$$\tilde{\phi}_R(x) = \begin{cases} \phi_R^{\mathrm{N}}(x) & \text{if } |x| \leq R/10, \\ \eta \lambda\left(\frac{|x| - R/10}{R}\right) & \text{if } |x| > R/10, \end{cases} \tag{2.9.7}$$

where η is chosen such that $\tilde{\phi}_R(x)$ is continuously differentiable, that is, $\eta = \phi_R^{\mathrm{N}}(eR/10)$ with $e \in \mathbb{R}^2$ a unit vector. We have

$$E_0 \leq \frac{\left\langle \tilde{\phi}_R, h\tilde{\phi}_R \right\rangle}{\left\langle \tilde{\phi}_R, \tilde{\phi}_R \right\rangle} = \frac{1}{\left\langle \tilde{\phi}_R, \tilde{\phi}_R \right\rangle} \left(E_R^{\mathrm{N}} + \frac{\eta^2}{R^2} \int_{|x| > R/10} \left| \lambda' \left(\frac{|x| - R/10}{R} \right) \right|^2 \mathrm{d}x \right). \tag{2.9.8}$$

With $|\lambda'(t)|^2 \leq 2$ and $\lambda'(t) = 0$ for $t \geq 1$ we see that the second integral on the right-hand side of Eq. (2.9.8) is bounded from above by $12\pi R^2/5$. We therefore have

$$E_R^{\mathrm{N}} \geq E_0 \left\|\tilde{\phi}_R\right\|^2 - \frac{12\pi}{5}\eta^2. \tag{2.9.9}$$

With the definition of λ we conclude

$$\left\|\tilde{\phi}_R\right\|^2 \leq 1 + 2\pi\eta^2 \int_{R/10}^{R/10+R} r\,\mathrm{d}r = 1 + \frac{6\pi}{5}\eta^2 R^2 \tag{2.9.10}$$

and since $E_0 < 0$, we have

$$E_R^{\mathrm{N}} \geq E_0 \left(1 + \frac{6\pi}{5}\eta^2 R^2\right) - \frac{12\pi}{5}\eta^2. \tag{2.9.11}$$

It remains to derive upper bounds for η and $|E_0|$.

Since ϕ_R^{N} is symmetrically decreasing and has L^2-norm equal to one its value at the boundary $\{x : |x| = R/10\}$ is at most $(\pi(R/10)^2)^{-1/2}$, that is, $\eta \leq 10/(\sqrt{\pi}R)$. On the other hand, we know from [74, Theorem 3.4] that

$$E_0 \sim -\frac{1}{R_0^2} \exp\left(\frac{-4\pi}{\frac{1}{R_0^2 \ln(R/R_0)} \int_{\mathbb{R}^2} \theta\,(R_0 - |x|)\,\mathrm{d}x}\right). \tag{2.9.12}$$

Here $E_0 \sim -\exp(-b/\delta)$ means that for all $\epsilon > 0$ there exists a $\delta_0 > 0$ such that $\exp(-(b + \epsilon)/\delta) \leq -E_0 \leq \exp(-(b - \epsilon)/\delta)$ for all $0 < \delta < \delta_0$. Together with Eq. (2.9.11) and the upper bound on η, this shows that for all $\epsilon > 0$ there exists a $\delta_0 > 0$ such that

$$E_R^{\mathrm{N}} \geq -\frac{121}{R^2}\left(\frac{R_0}{R}\right)^{2-\epsilon} - \frac{240}{R^2} \tag{2.9.13}$$

holds as long as $R_0/R < \delta_0$.

If this is not the case we use the simple bound

$$E_R^{\mathrm{N}} \geq -\frac{1}{R_0^2 \ln(R/R_0)}. \tag{2.9.14}$$

Since $R_0 < R/10$ by assumption we know that $\ln(R/R_0) > \ln(10)$. On the other hand, $R_0^2 \geq R^2\delta_0^2$ implies that

$$E_R^{\mathrm{N}} \geq -\frac{1}{R^2\delta_0^2 \ln(10)} \tag{2.9.15}$$

for $R_0/R \geq \delta_0$. This proves the claim (2.9.4). □

Note that for the simple step function potential in Lemma 5 we can also compute the scaling behavior of the lowest eigenvalue explicitly in terms of Bessel functions (see Section 1.6) or via the Sobolev inequality in two dimensions. The method of proof given here is more general, however.

Recall that $d(x_i, x_k) \geq R/5$ for $i, k \in J_j$. With $\tilde{U}_R(t) \leq j(0)/(R^2 \ln(R/\tilde{a})) = 8/(R^2 \ln(R/\tilde{a}))$, as well as using $\tilde{a} < R_0$, we see that Lemma 5 implies

$$\begin{aligned}
\left(\tilde{U}_R - U_R\right)\left(d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right) &\leq \theta\left(R_0 - d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right) \frac{8}{R^2 \ln(\tilde{a}/R)} \\
&= 8\left(\frac{R_0}{R}\right)^2 \sum_{i \in J_j} \theta\left(R_0 - d\left(x_i, x_j\right)\right) \frac{1}{R_0^2 \ln(\tilde{a}/R)} \\
&\leq 8\left(\frac{R_0}{R}\right)^2 \left[-\Delta_j + \frac{\tilde{C}}{R^2} \sum_{i \in J_j} \theta\left(R/10 - d(x_i, x_j)\right)\right] \\
&= 8\left(\frac{R_0}{R}\right)^2 \left[-\Delta_j + \frac{\tilde{C}}{R^2} \theta\left(R/10 - d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right)\right].
\end{aligned} \tag{2.9.16}$$

The constant $\tilde{C} > 0$ is determined by Lemma 5. On the other hand, we have that $\tilde{U}_R(t)$ can be bounded from below as $\tilde{U}_R(t) \geq j(1/10)/(R^2 \ln(R/\tilde{a}))$ for $t \leq R/10$ and this implies

$$\theta\left(R/10 - d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right) \leq \frac{\tilde{U}_R\left(d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right) R^2 \ln(R/\tilde{a})}{j(1/10)}. \tag{2.9.17}$$

Eqs. (2.9.16) and (2.9.17) together show that

$$\begin{aligned}
&\left(\tilde{U}_R - U_R\right)\left(d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right) \\
&\quad \leq -8\left(\frac{R_0}{R}\right)^2 \Delta_j + \frac{8\tilde{C}}{j(1/10)} \left(\frac{R_0}{R}\right)^2 \ln(R/\tilde{a}) \tilde{U}_R\left(d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right).
\end{aligned} \tag{2.9.18}$$

Define a' by the equation (assuming that the last factor on the right side is positive)

$$\frac{1}{\ln(R/a')} = \frac{1}{\ln(R/\tilde{a})}(1-\epsilon)(1-\kappa)\left(1 - \frac{8\tilde{C}}{j(1/10)}\left(\frac{R_0}{R}\right)^2 \ln(R/\tilde{a})\right) \tag{2.9.19}$$

and let

$$\tilde{U}'_R(t) = \frac{j(t/R)}{R^2 \ln(R/a')}. \tag{2.9.20}$$

We also define

$$\kappa' = \kappa - 8\left(\frac{R_0}{R}\right)^2 \tag{2.9.21}$$

and write the remaining kinetic energy as (compare with (2.8.7))

$$\begin{aligned} &-\nabla_j(1-(1-\kappa)\chi(p)^2)\nabla_j + (1-\epsilon)(1-\kappa)\left(8\left(\frac{R_0}{R}\right)^2\Delta_j\right) \\ &\geq -\nabla_j(1-(1-\kappa)\chi(p)^2)\nabla_j + 8\left(\frac{R_0}{R}\right)^2\Delta_j \\ &= -\Delta_j\kappa' - (1-\kappa)\nabla_j\left(1-\chi(p)^2\right)\nabla_j. \end{aligned} \tag{2.9.22}$$

In the following, we will choose $\kappa \gg R_0^2/R^2$, which, in particular, implies $\kappa' > 0$. Concerning the attractive part of the interaction potential that we obtain after applying Lemma 4, we use the definition of U_R to see that

$$\int_{\mathbb{R}_+} U_R(t)t\,\mathrm{d}t \leq \frac{1}{\ln(R/\tilde{a})}. \tag{2.9.23}$$

Eqs. (2.8.7), (2.9.18), (2.9.22) and (2.9.23) then imply

$$\mathbb{T} + \mathbb{V} \geq \mathbb{T}^{\mathrm{c}} + \mathbb{W}, \tag{2.9.24}$$

where

$$\mathbb{T}^{\mathrm{c}} = \sum_p \epsilon(p) a_p^\dagger a_p \quad \text{and} \quad \epsilon(p) = \kappa' p^2 + (1-\kappa)p^2\left(1-\chi(p)^2\right) - \mu_0. \tag{2.9.25}$$

In the Fock space sector with particle number n, the operator $\mathbb{W}$ is given by the (symmetrization of the) multiplication operator

$$\sum_{j=1}^n \left[\tilde{U}_R'\left(d\left(x_j, x_{\mathrm{NN}}^{J_j}\left(x_j\right)\right)\right) - \frac{1}{\epsilon\ln(R/\tilde{a})}\sum_{i\in J_j} w_R(x_j - x_i)\right]. \tag{2.9.26}$$

We note again that the set J_j depends on all particle coordinates x_i, $i \neq j$.

We conclude this section with the choice of the cutoff function χ. Let $\zeta : \mathbb{R}^2 \to \mathbb{R}_+$ be a smooth radial function with $\zeta(p) = 0$ for $|p| \leq 1$, $\zeta(p) = 1$ for $p \geq 2$, and $0 \leq \zeta(p) \leq 1$ in-between. For some $s \geq R$ we choose

$$\chi(p) = \zeta(sp). \tag{2.9.27}$$

We will choose $p_{\mathrm{c}} \leq 1/s$ below. This implies in particular that $\epsilon(p) = (1-\kappa+\kappa')p^2 - \mu_0$ for $|p| < p_{\mathrm{c}}$. We therefore have

$$\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{T}^{\mathrm{c}}\Upsilon_\pi^z\right] = \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{T}^{\mathrm{c}}\Upsilon^z\right] + \sum_{|p|<p_{\mathrm{c}}}\left((1-\kappa+\kappa')p^2 - \mu_0\right)\pi_p. \tag{2.9.28}$$

Using Eqs. (2.7.9), (2.9.24), (2.9.28) and further

$$\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{T}^{\mathrm{c}}\Upsilon^{z}\right] - \frac{1}{\beta} S\left(\Upsilon^{z}\right) \geq -\frac{1}{\beta} \ln \mathrm{Tr}_{\mathcal{F}_{>}} \exp\left(-\beta \mathbb{T}_{\mathrm{s}}^{\mathrm{c}}(z)\right), \tag{2.9.29}$$

we conclude that

$$\begin{aligned} F_z(\beta) \geq & -\frac{1}{\beta} \ln \mathrm{Tr}_{\mathcal{F}_{>}} \exp\left(-\beta \mathbb{T}_{\mathrm{s}}^{\mathrm{c}}(z)\right) + \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}\Upsilon_{\pi}^{z}\right] + \tfrac{1}{2} \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{K}\Upsilon^{z}\right] \\ & - (\kappa - \kappa') \sum_{|p|<p_{\mathrm{c}}} p^2 \pi_p - Z^{(2)}. \end{aligned} \tag{2.9.30}$$

The first term on the right-hand side of (2.9.30) can be computed explicitly and reads

$$\begin{aligned} & -\frac{1}{\beta} \ln \mathrm{Tr}_{\mathcal{F}_{>}} \exp\left(-\beta \mathbb{T}_{\mathrm{s}}^{\mathrm{c}}(z)\right) \\ & = \sum_{|p|<p_{\mathrm{c}}} \Big((1 - \kappa + \kappa')\, p^2 - \mu_0 \Big) |z_p|^2 + \frac{1}{\beta} \sum_{|p| \geq p_{\mathrm{c}}} \ln\left(1 - \exp\left(-\beta \epsilon(p)\right)\right). \end{aligned} \tag{2.9.31}$$

In the following, we will derive a lower bound on $\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}\Upsilon_{\pi}^{z}\right]$.

2.10 Localization of relative entropy

In order to compute $\mathrm{Tr}_{\mathcal{F}}[\mathbb{W}\Upsilon_{\pi}^{z}]$ we will replace the unknown state Γ^{z} in the definition of $\Upsilon_{\pi}^{z} = U(z)\Pi U(z)^{\dagger} \otimes \Gamma^{z}$ by the quasi-free state Γ_0, the Gibbs state for the kinetic energy operator $\mathbb{T}_{\mathrm{s}}(z)$. The error resulting from this replacement will be controlled via the a priori bound on the relative entropy (2.6.4). For that purpose we need a local version of the relative entropy bound, which will be derived in this section.

Let us denote by Ω_π the quasi-free state whose one-particle density matrix is given by

$$\omega_\pi = \sum_p \omega_\pi(p) |p\rangle\langle p| = \sum_p \frac{1}{\mathrm{e}^{\ell(p)} - 1} |p\rangle\langle p|, \tag{2.10.1}$$

where

$$\ell(p) = \begin{cases} \ln(1 + 1/\pi_p) & \text{if } |p| < p_{\mathrm{c}}, \\ \beta(p^2 - \mu_0) & \text{if } |p| \geq p_{\mathrm{c}}. \end{cases} \tag{2.10.2}$$

In other words,

$$\Omega_\pi = \Pi \otimes \Gamma_0. \tag{2.10.3}$$

We will choose π_p such that $\ell(p) \geq \beta(p^2 - \mu_0)$ holds for all p. Let $\eta : \mathbb{R}_+ \to [0, 1]$ be a function with the following properties:

- $\eta \in C^\infty(\mathbb{R}_+)$
- $\eta(0) = 1$, and $\eta(x) = 0$ for $x \geq 1$
- $\hat{\eta}(p) = \int_{\mathbb{R}^2} \eta(|x|)\, \mathrm{e}^{-ipx}\, \mathrm{d}x \geq 0$ for all $p \in \mathbb{R}^2$.

Such a function can be obtained by choosing a smooth radial and nonnegative function on $\mathbb{R}^2$ with compact support and then convolving it with itself. Given a function with these properties, we define $\eta_b(x) = \eta(x/b)$ for some $b \leq L/2$. We also define the one-particle density matrix ω_b be defined by its integral kernel

$$\omega_b(x, y) = \omega_\pi(x, y)\eta_b(d(x, y)). \tag{2.10.4}$$

The unique quasi-free state related to ω_b will be denoted by Ω_b and we define

$$\Omega_b^z = U(z)\Omega_b U(z)^\dagger. \tag{2.10.5}$$

We also introduce $\rho_\omega = \omega_b(x, x) = \omega_\pi(x, x)$.

To state the inequality we are looking for, we need to define spatial restriction of states. To that end, we denote for $r < L/2$ by $\chi_{r,\xi}(x) = \theta(r - d(x, \xi))$ the characteristic function of a disk of radius r centered at $\xi \in \Lambda$. Since $\chi_{r,\xi}$ defines a projection on the one-particle Hilbert space $\mathcal{H} = L^2(\Lambda)$, the Fock space $\mathcal{F}$ over $\mathcal{H}$ is unitarily equivalent to the product of two Fock spaces

$$\mathcal{F}(\mathcal{H}) \cong \mathcal{F}(\chi_{r,\xi}\mathcal{H}) \otimes \mathcal{F}((\chi_{r,\xi}\mathcal{H})^\perp). \tag{2.10.6}$$

Any state on $\mathcal{F}$ can be restricted to the Fock space over $\chi_{r,\xi}\mathcal{H}$ by taking the partial trace over the second tensor factor in (2.10.6). The restriction of the state Γ will be denoted by $\Gamma_{\chi_{r,\xi}}$.

If $d(\xi, \zeta) > 2r$ the multiplication operator $\chi_{r,\xi} + \chi_{r,\zeta}$ defines a projection and using the fact that $\omega_b(x, y) = 0$ as long as $d(x, y) > b$ we easily check that

$$\Omega_{b,\chi_{r,\xi}+\chi_{r,\zeta}} \cong \Omega_{b,\chi_{r,\xi}} \otimes \Omega_{b,\chi_{r,\zeta}} \tag{2.10.7}$$

holds if $d(\xi, \zeta) > 2r + b$. More precisely, we use that the one-particle density matrix of $\Omega_{b,\chi_{r,\xi}+\chi_{r,\zeta}}$ is given by $(\chi_{r,\xi} + \chi_{r,\zeta})\omega_b(\chi_{r,\xi} + \chi_{r,\zeta}) = \chi_{r,\xi}\omega_b\chi_{r,\xi} + \chi_{r,\zeta}\omega_b\chi_{r,\zeta}$. The right-hand side is nothing else but the one-particle density matrix of $\Omega_{b,\chi_{r,\xi}}$ plus the one of $\Omega_{b,\chi_{r,\zeta}}$, which proves the claim. The above identity also holds for Ω_b^z because $U(z)$ has the same product structure.

Concerning spatial localization, the relative entropy is superadditive in the following sense.

Lemma 6. *Let X_i, $1 \le i \le k$, denote k mutually orthogonal projections on $\mathcal{H}$. Let Ω be a state on $\mathcal{F}$ which factorizes under restrictions as $\Omega_{\sum_i X_i} = \otimes_i \Omega_{X_i}$. Then, for any state Γ, we have*

$$S(\Gamma, \Omega_{\sum_i X_i}) \ge \sum_i S(\Gamma_{X_i}, \Omega_{X_i}). \tag{2.10.8}$$

The proof of Lemma 6 can be found in [70, Section 2.8], see also [68, Section 5.1]. We emphasize that the factorization property of Ω is crucial, the relative entropy need not be superadditive, in general. This is the reason for introducing the cutoff b. Without it, the state Ω_b^z would not factorize as in (2.10.7).

We apply Lemma 6 with $\Omega = \Omega_b^z$ and X_i multiplication operators of characteristic functions of balls with radius r that are separated by a distance $2b$. When we average over the position of the balls (see [68, Section 5.1] for details), we obtain for $r \le 2b$ and $L/(2b) \in \mathbb{N}$ the inequality

$$S(\Gamma, \Omega_b^z) \ge \frac{1}{(2b)^2} \int_\Lambda S\left(\Gamma_{\chi_{r,\xi}}, \Omega^z_{b,\chi_{r,\xi}}\right) \mathrm{d}\xi. \tag{2.10.9}$$

That is, the integral over local relative entropies of Γ with respect to Ω_b^z can be estimated from above by their global relative entropy. The restriction $L/(2b) \in \mathbb{N}$ is of no further importance since we take the thermodynamic limit. From (2.10.9) for $\Gamma = \Upsilon_\pi^z$, we infer

$$\begin{aligned}
\int_\Lambda \left\| \Upsilon^z_{\pi,\chi_{r,\xi}} - \Omega^z_{b,\chi_{r,\xi}} \right\|_1 \mathrm{d}\xi &\le |\Lambda|^{1/2} \left(\int_\Lambda \left\| \Upsilon^z_{\pi,\chi_{r,\xi}} - \Omega^z_{b,\chi_{r,\xi}} \right\|_1^2 \mathrm{d}\xi \right)^{1/2} \\
&\le \sqrt{2} |\Lambda|^{1/2} \left(\int_\Lambda S(\Upsilon^z_{\pi,\chi_{r,\xi}}, \Omega^z_{b,\chi_{r,\xi}}) \, \mathrm{d}\xi \right)^{1/2} \\
&\le 2^{3/2} b |\Lambda|^{1/2} S(\Upsilon_\pi^z, \Omega_b^z)^{1/2}
\end{aligned} \tag{2.10.10}$$

for any $b \ge 2r$. This estimate follows from using the Cauchy-Schwarz inequality for the integral over ξ and the fact that the relative entropy of two states Γ and Γ' is bounded from below by the square of the trace norm distance, by Pinsker's inequality (see [60, Theorem 1.15]),

$$S(\Gamma, \Gamma') \ge \frac{1}{2} \|\Gamma - \Gamma'\|_1^2. \tag{2.10.11}$$

In Section 2.15, we will estimate the effect of the cutoff b and obtain a bound on (2.10.10) in terms of the a priori bound (2.6.4) on the relative entropy. We remark that Pinsker's inequality could not be used with benefit for the global relative entropy. This is because the relative entropy is an extensive quantity while the trace norm difference of two states is always bounded by two.

2.11 Interaction energy, part I

In the following three subsections we shall derive a lower bound on $\mathrm{Tr}_{\mathcal{F}}[\mathbb{W}\Upsilon_\pi^z]$. The estimate (2.10.10) will play an important role in this analysis. We start by giving a bound on the first term in (2.9.26) in this section, and postpone the analysis of the second term to Section 2.12. In Section 2.13 we combine these bounds to obtain the final bound. A main difficulty is related to the fact that the vector z is rather arbitrary, and hence the density of the particles described by the coherent states can be far from homogeneous.

Let us give a name to the positive and the negative part of the interaction energy. We write

$$\mathbb{W} = \mathbb{W}_1 - \mathbb{W}_2, \tag{2.11.1}$$

where

$$\mathbb{W}_1 = \bigoplus_{n=0}^{\infty} \sum_{j=1}^{n} \tilde{U}'_R \left(d\left(x_j, x_{\mathrm{NN}}^{J_j}(x_j)\right)\right) \tag{2.11.2}$$

and

$$\mathbb{W}_2 = \bigoplus_{n=0}^{\infty} \sum_{j=1}^{n} \sum_{i\in J_j} \frac{1}{\epsilon \ln(R/\tilde{a})} w_R(x_j - x_i). \tag{2.11.3}$$

We start by giving a lower bound to the expectation of $\mathbb{W}_1$ in the state Υ_π^z. First of all, recalling the definition of j from (2.9.1), we note that since $L \geq 2R$ we can write

$$j(d(x,y)/R) = \frac{32}{\pi R^2} \int_\Lambda \theta(R/2 - d(\xi, x))\theta(R/2 - d(\xi, y))\, \mathrm{d}\xi \tag{2.11.4}$$

for $x, y \in \Lambda$. Inserting this into (2.9.20), we have

$$\tilde{U}'_R\,(d(x,y)) = \frac{32}{\pi \ln(R/a')R^4} \int_\Lambda \theta(R/2 - d(\xi, x))\theta(R/2 - d(\xi, y))\, \mathrm{d}\xi. \tag{2.11.5}$$

This gives rise to a similar decomposition of $\mathbb{W}_1$ which we write as

$$\mathbb{W}_1 = \frac{32}{\pi \ln(R/a')R^4} \int_\Lambda w(\xi)\, \mathrm{d}\xi, \tag{2.11.6}$$

with

$$w(\xi) = \bigoplus_{n=0}^{\infty} \sum_{j=1}^{n} \theta\left(R/2 - d\left(\xi, x_j\right)\right) \theta\left(R/2 - d\left(\xi, x_{\mathrm{NN}}^{J_j}(x_j)\right)\right). \tag{2.11.7}$$

For $r > 0$, define $n_{r,\xi}$ as the number operator of a ball of radius r centered at $\xi \in \Lambda$, which is nothing else but the second quantization of the multiplication operator $\theta(r - d(\xi, \cdot))$ on $L^2(\Lambda)$. We claim

$$w(\xi) \geq n_{R/10,\xi}\theta(n_{R/10,\xi} - 2), \tag{2.11.8}$$

which is the second quantized version of

$$\theta(R/2 - d(\xi, x_j))\theta\left(R/2 - d\left(\xi, x_{\mathrm{NN}}^{J_j}(x_j)\right)\right) \geq \theta(R/10 - d(\xi, x_j))\left(1 - \prod_{i \neq j} \theta(d(\xi, x_i) - R/10)\right), \tag{2.11.9}$$

which can be shown using the defining property of J_j. More precisely, (2.11.9) says that if x_j and some x_k with $k \neq j$ are in a disk of radius $R/10$ centered at ξ (i.e., if the right-hand side is equal to one), then the nearest neighbor of x_j in the set J_j is in a disk of radius $R/2$ with the same center (i.e., the left-hand side equals one). Assume therefore that x_j and x_k are in a disk of radius $R/10$ centered at ξ and $k \in J_j$. Then we have

$$d\left(x_j, x_{\mathrm{NN}}^{J_j}(x_j)\right) \leq d(x_j, x_k) \leq \frac{R}{5}, \tag{2.11.10}$$

which implies $d(\xi, x_{\mathrm{NN}}^{J_j}(x_j)) \leq 3R/10$. Conversely, if $k \notin J_j$, then by definition of J_j, there exists $l \in J_j$ such that $d(x_l, x_k) < R/5$. Therefore

$$d\left(x_j, x_{\mathrm{NN}}^{J_j}(x_j)\right) \leq d(x_j, x_l) < \frac{2R}{5}, \tag{2.11.11}$$

which implies $d(\xi, x_{\mathrm{NN}}^{J_j}(x_j)) < R/2$ and proves (2.11.9).

In particular, the above implies

$$w(\xi) \geq \overline{w}(\xi) := w(\xi)\theta\left(2 - n_{3R/2,\xi}\right) + n_{R/10,\xi}\theta\left(n_{R/10,\xi} - 2\right)\theta\left(n_{3R/2,\xi} - 3\right). \tag{2.11.12}$$

We also have

$$w(\xi)\theta\left(2 - n_{3R/2,\xi}\right) = n_{R/2,\xi}\left(n_{R/2,\xi} - 1\right)\theta\left(2 - n_{3R/2,\xi}\right), \tag{2.11.13}$$

which can be seen from the following consideration. Assume two particles x_i and x_j are in a disk of radius $R/2$ and no other particle is in the bigger disk of radius $3R/2$ (with the same center), then these two particles must be nearest neighbors and by construction $i \in J_j$ and $j \in J_i$, which implies (2.11.13).

We note that the operator in (2.11.13) is bounded. Its operator norm equals two and in combination with $n_{R/10,\xi} \leq n_{3R/2,\xi}$, this implies that

$$|\overline{w}(\xi) - n_{R/10,\xi}| \leq 2, \tag{2.11.14}$$

as can be seen using (2.11.12) and an easy counting argument. Eqs. (2.11.6), (2.11.12) and (2.11.14) imply that

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}_1 \Upsilon_\pi^z\right] &\geq \frac{32}{\pi \ln(R/a')R^4} \int_\Lambda \mathrm{Tr}_{\mathcal{F}}\left[\overline{w}(\xi)\Upsilon_\pi^z\right] \mathrm{d}\xi \\ &\geq \frac{32}{\pi \ln(R/a')R^4} \int_\Lambda \mathrm{Tr}_{\mathcal{F}}\left[\overline{w}(\xi)\Omega_b^z + n_{R/10,\xi}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right] \mathrm{d}\xi \\ &\quad - \frac{64}{\pi \ln(R/a')R^4} \int_\Lambda \left\| \Upsilon^z_{\pi,\chi_{3R/2,\xi}} - \Omega^z_{b,\chi_{3R/2,\xi}} \right\|_1 \mathrm{d}\xi. \end{aligned} \tag{2.11.15}$$

The second term on the right-hand side of (2.11.15) can be written as

$$\int_\Lambda \mathrm{Tr}_{\mathcal{F}}\left[n_{R/10,\xi}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right] \mathrm{d}\xi = \pi \left(\frac{R}{10}\right)^2 \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right]. \tag{2.11.16}$$

On the other hand, Eq. (2.10.10) implies that

$$\int_\Lambda \left\| \Upsilon^z_{\pi,\chi_{3R/2,\xi}} - \Omega^z_{b,\chi_{3R/2,\xi}} \right\|_1 \mathrm{d}\xi \leq 2^{3/2} b |\Lambda|^{1/2} S(\Upsilon_\pi^z, \Omega_b^z)^{1/2} \tag{2.11.17}$$

holds as long as $3R \leq b$.

In the following we will derive two different lower bounds to $\mathrm{Tr}_{\mathcal{F}}[\overline{w}(\xi)\Omega_b^z]$ in order to have a good bound for all values of z. To obtain the first bound, we use (2.11.12) (where we drop the last term for a lower bound) and (2.11.13). This implies

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\left[\overline{w}(\xi)\Omega_b^z\right] \geq \Big[& \mathrm{Tr}_{\mathcal{F}}\left[n_{R/2,\xi}\left(n_{R/2,\xi} - 1\right)\Omega_b^z\right] \\ & - \mathrm{Tr}_{\mathcal{F}}\left[n_{3R/2,\xi}\left(n_{3R/2,\xi} - 1\right)\left(n_{3R/2,\xi} - 2\right)\Omega_b^z\right]\Big]_+, \end{aligned} \tag{2.11.18}$$

where we take the positive part of this bound since the right-hand side can become negative, in which case we simply estimate the left-hand side by zero. The advantage of the right-hand side of (2.11.18) is that all terms can be evaluated explicitly because Ω_b^z is a combination of a coherent and a quasi-free state. Let Φ_z denote the one-particle wave function $|\Phi_z\rangle = \sum_{|p|<p_c} z_p |p\rangle$. We write

$$n_{3R/2,\xi} = \int_{B_{3R/2}(\xi)} a_x^\dagger a_x \,\mathrm{d}x. \tag{2.11.19}$$

By abuse of notation, we use the same letter for the plane wave expansion of the creation/annihilation operators, given by

$$a_x := \frac{1}{L} \sum_p a_p \,\mathrm{e}^{ipx}, \tag{2.11.20}$$

and analogously for $a_x^\dagger$. The following identity is a direct consequence of (2.11.19) and the canonical commutation relations:

$$n_{3R/2,\xi}\left(n_{3R/2,\xi}-1\right)\left(n_{3R/2,\xi}-2\right)=\int_{B_{3R/2}(\xi)^3} a_x^\dagger a_y^\dagger a_z^\dagger a_z a_y a_x \,\mathrm{d}(x,y,z). \tag{2.11.21}$$

We have

$$U(z)^\dagger a_x U(z)=a_x+\sum_{|p|<p_c} z_p\frac{\mathrm{e}^{ipx}}{L}=a_x+\Phi_z(x), \tag{2.11.22}$$

which means that conjugation by the unitary $U(z)$ shifts the annihilation operators by Φ_z. Inserting this as well as (2.11.21) we have

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}&\left[n_{3R/2,\xi}\left(n_{3R/2,\xi}-1\right)\left(n_{3R/2,\xi}-2\right)\Omega_b^z\right]=\int_{B_{3R/2}(\xi)^3}\mathrm{d}(x,y,z)\\ &\times\left\langle(a_x^\dagger+\Phi_z^\dagger(x))(a_y^\dagger+\Phi_z^\dagger(y))(a_z^\dagger+\Phi_z^\dagger(z))(a_z+\Phi_z(z))(a_y+\Phi_z(y))(a_x+\Phi_z(x))\right\rangle_{\Omega_b}.\end{aligned} \tag{2.11.23}$$

Now we multiply out the terms in the expectation and use Wick's theorem. It is helpful to introduce the short hand notation $\bar{n}_x=\langle a_x^\dagger a_x\rangle_{\Omega_b}$. Renaming integration variables to collect similar terms, we arrive at

$$\begin{aligned}(2.11.23)=&\int_{B_{3R/2}(\xi)^3}\mathrm{d}(x,y,z)\left[\bar{n}_x\bar{n}_y\bar{n}_z+3\bar{n}_x|\Phi_z(y)|^2|\Phi_z(z)|^2+3\bar{n}_x\bar{n}_y|\Phi_z(z)|^2\right.\\ &+|\Phi_z(x)|^2|\Phi_z(y)|^2|\Phi_z(z)|^2+2\omega_b(x,y)\omega_b(y,z)\omega_b(z,x)+6\Phi_z^\dagger(x)\Phi_z(z)\omega_b(x,y)\omega_b(y,z)\\ &+6\bar{n}_x\Phi_z^\dagger(y)\Phi_z(z)\omega_b(y,z)+6|\Phi_z(x)|^2\Phi_z^\dagger(y)\Phi_z(z)\omega_b(y,z)\\ &\left.+3\bar{n}_x\omega_b(y,z)\omega_b(z,y)+3\,|\Phi_z(x)|^2\omega_b(y,z)\omega_b(z,y)\right].\end{aligned} \tag{2.11.24}$$

This can be rewritten as

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}&\left[n_{3R/2,\xi}\left(n_{3R/2,\xi}-1\right)\left(n_{3R/2,\xi}-2\right)\Omega_b^z\right] \qquad (2.11.25)\\ &=\left(\mathrm{Tr}_{\mathcal{F}}\left[n_{3R/2,\xi}\Omega_b^z\right]\right)^3+2\,\mathrm{tr}\left(\chi_{3R/2,\xi}\omega_b\right)^3+6\langle\Phi_z|\left(\chi_{3R/2,\xi}\omega_b\chi_{3R/2,\xi}\right)^2|\Phi_z\rangle\\ &\quad+3\,\mathrm{Tr}_{\mathcal{F}}\left[n_{3R/2,\xi}\Omega_b^z\right]\left(2\langle\Phi_z|\chi_{3R/2,\xi}\omega_b\chi_{3R/2,\xi}|\Phi_z\rangle+\mathrm{tr}\left(\chi_{3R/2,\xi}\omega_b\right)^2\right)\\ &\le 6\left(\mathrm{Tr}_{\mathcal{F}}\left[n_{3R/2,\xi}\Omega_b^z\right]\right)^3.\end{aligned}$$

Here the symbol tr denotes the trace over the one-particle Hilbert space $L^2(\Lambda)$. Therefore, the first lower bound is

$$\mathrm{Tr}_{\mathcal{F}}[\overline{w}(\xi)\Omega_b^z]\ge\left[\mathrm{Tr}_{\mathcal{F}}\left[n_{R/2,\xi}\left(n_{R/2,\xi}-1\right)\Omega_b^z\right]-6\left(\mathrm{Tr}_{\mathcal{F}}\left[n_{3R/2,\xi}\Omega_b^z\right]\right)^3\right]_+. \tag{2.11.26}$$

The second lower bound to $\mathrm{Tr}_{\mathcal{F}}[\overline{w}(\xi)\Omega_b^z]$ can be obtained using

$$\mathrm{Tr}_{\mathcal{F}}\left[\overline{w}(\xi)\Omega_b^z\right] \geq \mathrm{Tr}_{\mathcal{F}}\left[n_{R/10,\xi}\theta\left(n_{R/10,\xi}-2\right)\Omega_b^z\right], \tag{2.11.27}$$

which follows from (2.11.8). Let us denote by $\Pi_0^{\mathcal{F}}$ the vacuum state on $\mathcal{F}$. The state $\Omega_{b,\chi_{R/10,\xi}}$ is a particle number conserving quasi-free state, whose vacuum expectation is given by

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}(\chi_{R/10,\xi}\mathcal{H})}[\Omega_{b,\chi_{R/10,\xi}}\Pi^{\mathcal{F}}_{0,\chi_{R/10,\xi}}] &= \exp\left(-\operatorname{tr}\ln\left(1+\chi_{R/10,\xi}\omega_b\chi_{R/10,\xi}\right)\right)\\ &\geq \exp\left(-\operatorname{tr}\chi_{R/10,\xi}\omega_b\chi_{R/10,\xi}\right) = \exp\left(-\pi(R/10)^2\rho_\omega\right),\end{aligned} \tag{2.11.28}$$

where ρ_ω was defined after (2.10.5) to be the density of Ω_b. Hence,

$$\Omega_{b,\chi_{R/10,\xi}} \geq \exp\left(-\pi(R/10)^2\rho_\omega\right)\Pi^{\mathcal{F}}_{0,\chi_{R/10,\xi}}, \tag{2.11.29}$$

as well as

$$\Omega^z_{b,\chi_{R/10,\xi}} \geq \exp\left(-\pi(R/10)^2\rho_\omega\right)\left(U(z)\Pi_0^{\mathcal{F}}U(z)^\dagger\right)_{\chi_{R/10,\xi}}. \tag{2.11.30}$$

This in particular implies

$$\mathrm{Tr}_{\mathcal{F}}\left[\overline{w}(\xi)\Omega_b^z\right] \geq \mathrm{e}^{-\pi(R/10)^2\rho_\omega}\,\mathrm{Tr}_{\mathcal{F}}\left[n_{R/10,\xi}\theta\left(n_{R/10,\xi}-2\right)U(z)\Pi_0^{\mathcal{F}}U(z)^\dagger\right]. \tag{2.11.31}$$

The state $U(z)\Pi_0^{\mathcal{F}}U(z)^\dagger$ as well as its restriction to the Fock space over $\chi_{R/10,\xi}\mathcal{H}$ are coherent states. In the Fock space sector with n particles, the latter is given by the projection onto the n-fold tensor product of the wave function $\chi_{R/10,\xi}\Phi_z$ times a normalization factor. We therefore have

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}\left[n_{R/10,\xi}\theta\left(n_{R/10,\xi}-2\right)U(z)\Pi_0^{\mathcal{F}}U(z)^\dagger\right] &= \mathrm{e}^{-\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}\sum_{n\geq 2} n\frac{\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle^n}{n!}\\ = \langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle\left(1-\mathrm{e}^{-\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}\right) &\geq \frac{\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle^2}{1+\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}.\end{aligned} \tag{2.11.32}$$

To arrive at the last line, we used the estimate $x(1-e^{-x}) \geq x^2/(1+x)$ for $x \geq 0$.

Summarizing the results of this section, we combine the estimates from Eqs. (2.11.15), (2.11.17), (2.11.18), (2.11.25), (2.11.31) as well as (2.11.32) and have thus shown that for any $0 \leq \lambda \leq 1$,

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}_1\Upsilon_\pi^z\right] \geq{}& \frac{8}{25\ln(R/a')R^2}\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z-\Omega_b^z\right)\right] - \frac{128\sqrt{2}b|\Lambda|^{1/2}}{\pi\ln(R/a')R^4}S(\Upsilon_\pi^z,\Omega_b^z)^{1/2}\\ &+ \frac{32\lambda}{\pi\ln(R/a')R^4}\int_\Lambda\left[\mathrm{Tr}_{\mathcal{F}}\left[n_{R/2,\xi}\left(n_{R/2,\xi}-1\right)\Omega_b^z\right] - 6\left(\mathrm{Tr}_{\mathcal{F}}\left[n_{3R/2,\xi}\Omega_b^z\right]\right)^3\right]_+\mathrm{d}\xi\\ &+ \frac{32(1-\lambda)\,\mathrm{e}^{-\pi(R/10)^2\rho_\omega}}{\pi\ln(R/a')R^4}\int_\Lambda\frac{\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle^2}{1+\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}\mathrm{d}\xi.\end{aligned} \tag{2.11.33}$$

The choice of λ will depend on the function $|\Phi_z|$. If it is approximately a constant, in a sense to be defined in Section 2.13 below, we will choose $\lambda = 1$, otherwise we choose $\lambda = 0$.

2.12 Interaction energy, part II

In this section we give an upper bound on the expectation value of $\mathbb{W}_2$ in (2.11.3). The two-dimensional version of [70, Lemma 5] is the following statement[3].

Lemma 7. *Let $o : \mathbb{R}^2 \to \mathbb{C}$ be a smooth function, supported in a cube of side length 4, and for $s > 0$, let $u(x) = |\Lambda|^{-1} \sum_p o(sp)\,\mathrm{e}^{-ipx}$. Then for any nonnegative integer n there exists a constant C_n such that*

$$|u(x)| \leq \left(\frac{s}{d(x,0)}\right)^{2n} C_n \max_{|\alpha|=2n} \|\partial^\alpha o\|_\infty \left(\frac{2}{\pi s} + \frac{2n+1}{L}\right)^2. \tag{2.12.1}$$

Here $\partial^\alpha o$ denotes the partial derivative of o with respect to the multiindex α.

Proof. For $x \in \mathbb{R}^2$ we write $x = (x_1, x_2)$. We have

$$\begin{aligned}
&u(x)L^2\left(4 - 2\cos\left(\frac{2\pi x_1}{L}\right) - 2\cos\left(\frac{2\pi x_2}{L}\right)\right) \\
&\quad= \sum_p o(sp)\,\mathrm{e}^{-ipx}\left(4 - \mathrm{e}^{i2\pi x_1/L} - \mathrm{e}^{-i2\pi x_1/L} - \mathrm{e}^{i2\pi x_2/L} - \mathrm{e}^{-i2\pi x_2/L}\right) \\
&\quad= \sum_p o(sp)\left(4\,\mathrm{e}^{-ipx} - \mathrm{e}^{-i(p_1-2\pi/L)x_1-ip_2x_2} - \mathrm{e}^{-i(p_1+2\pi/L)x_1-ip_2x_2}\right. \\
&\qquad\quad \left. - \mathrm{e}^{-ip_1x_1-i(p_2-2\pi/L)x_2} - \mathrm{e}^{-ip_1x_1-i(p_2+2\pi/L)x_2}\right) \\
&\quad= \sum_p \mathrm{e}^{-ipx}\left(4o(sp) - o(s(p_1+2\pi/L), sp_2) - o(s(p_1-2\pi/L), sp_2)\right. \\
&\qquad\quad \left. - o(sp_1, s(p_2+2\pi/L)) - o(sp_1, s(p_2-2\pi/L))\right) \\
&\quad= \frac{1}{|\Lambda|}\sum_p \mathrm{e}^{-ipx}(-\Delta_{\mathrm{d}})[o(sp)],
\end{aligned} \tag{2.12.2}$$

[3] In [70, proof of Lemma 5] it is claimed that the discrete Laplacian can be bounded by the continuous one with constant one, which is not correct, since also the mixed derivatives have to be taken into account. The correct version of that estimate is given in (2.12.4) below.

where $(-\Delta_{\mathrm{d}})f(p) = L^2(4f(p) - \sum_{|e|=1} f(p + 2\pi e/L))$ denotes the discrete Laplacian in momentum space. Therefore,

$$u(x)\left(2L^2\left(2-\cos\left(\frac{2\pi x_1}{L}\right)-\cos\left(\frac{2\pi x_2}{L}\right)\right)\right)^n = \frac{1}{|\Lambda|}\sum_p \mathrm{e}^{-ipx}(-\Delta_{\mathrm{d}})^n[o(sp)]. \qquad (2.12.3)$$

It is easy to check that the discrete Laplacian can be estimated by maximizing over the second partial derivatives as

$$|(-\Delta_{\mathrm{d}})^n f(p)| \leq C_n \max_{|\alpha|=2n} \|\partial^\alpha f\|_\infty \qquad (2.12.4)$$

for an n-dependent constant C_n independent of f. Note also that if f is supported in a square of side length ℓ, then after n-fold application of $-\Delta_{\mathrm{d}}$ the support is contained in a square of side length $\ell + 4\pi n/L$. An easy counting argument then allows us to estimate

$$\begin{aligned} |(2.12.3)| &\leq \frac{C_n}{|\Lambda|} \max_{|\alpha|=2n} \|\partial^\alpha o(s\,\cdot)\|_\infty \sum_p \mathbb{1}_{\mathrm{supp}(-\Delta_{\mathrm{d}})^n o(sp)} \\ &\leq \frac{C_n s^{2n}}{|\Lambda|} \max_{|\alpha|=2n} \|\partial^\alpha o\|_\infty \left(1 + \frac{2L}{\pi s} + 2n\right)^2 \\ &= C_n s^{2n} \max_{|\alpha|=2n} \|\partial^\alpha o\|_\infty \left(\frac{2}{\pi s} + \frac{2n+1}{L}\right)^2. \end{aligned} \qquad (2.12.5)$$

We also estimate

$$1 - \cos\left(\frac{2\pi x_i}{L}\right) \geq \frac{8}{L^2} \min_{k\in\mathbb{Z}} |x_i - kL|^2 \qquad (2.12.6)$$

and obtain

$$2L^2\left(2-\cos\left(\frac{2\pi x_1}{L}\right)-\cos\left(\frac{2\pi x_2}{L}\right)\right) \geq 16 d(x,0)^2. \qquad (2.12.7)$$

Absorbing the factor 16 into the constant C_n, we arrive at (2.12.1) and have completed the proof. □

We note that (by the definition of f_R in (2.8.2))

$$f_R(x) \leq R \sup_{d(x,y)\leq R} |\nabla h(y)| \leq R \sup_{d(x,y)\leq s} |\nabla h(y)|, \qquad (2.12.8)$$

where we used $R \leq s$ and conclude by applying Lemma 7 to ∇h that there exists a smooth function g of rapid decay (i.e., g decays like an arbitrary power) that is independent of L for large L such that the function w_R defined in (2.8.2) satisfies

$$w_R(x-y) \leq \frac{R^2}{s^4} g(d(x,y)/s). \qquad (2.12.9)$$

For $\mathbb{W}_2$ this implies

$$\mathbb{W}_2 \leq \bigoplus_{n=0}^{\infty} \sum_{j=1}^{n} \sum_{i \in J_j} \frac{1}{\epsilon \ln(R/\tilde{a})} \frac{R^2}{s^4} g\left(\frac{d(x_j, x_i)}{s}\right). \tag{2.12.10}$$

Next we decompose the function g into an integral over characteristic functions of balls. For this purpose, we use [31, Theorem 1] which allows us to write

$$g(t) = \int_0^{\infty} m(r) j(t/r)\, \mathrm{d}r \tag{2.12.11}$$

with

$$m(r) = -\frac{r}{16} \int_r^{\infty} g'''(s) s \left(s^2 - r^2\right)^{-1/2} \mathrm{d}s \tag{2.12.12}$$

and j defined in (2.9.1). Since the third derivative of g, denoted here by g''', is of rapid decay, the same is true for m. As j is a decreasing function, we have

$$g(t) \leq j(t) \int_0^1 |m(r)|\, \mathrm{d}r + \int_1^{\infty} |m(r)| j(t/r)\, \mathrm{d}r, \tag{2.12.13}$$

which implies

$$\begin{aligned} g\left(\frac{d(x_i, x_j)}{s}\right) \leq & \left(\int_0^1 |m(r)|\, \mathrm{d}r\right) \int_s^{\infty} j\left(\frac{d(x_i, x_j)}{r}\right) \delta(r - s)\, \mathrm{d}r \\ & + s^{-1} \int_s^{\infty} |m(r/s)| j\left(\frac{d(x_i, x_j)}{r}\right) \mathrm{d}r. \end{aligned} \tag{2.12.14}$$

Note that the integral over the δ function is understood as evaluation at $r = s$. As noted before in (2.11.4), we can write

$$j(d(x_i, x_j)/r) = \frac{32}{\pi r^2} \int_{\Lambda} \chi_{r/2,\xi}(x_i) \chi_{r/2,\xi}(x_j)\, \mathrm{d}\xi \tag{2.12.15}$$

as long as $L \geq 2r$. Eqs. (2.12.10) and (2.12.14) together with Eq. (2.12.15) show that

$$\begin{aligned} \mathbb{W}_2 \leq & \frac{32}{\pi \epsilon \ln(R/\tilde{a})} \frac{R^2}{s^6} \int_s^b \mathrm{d}r \left\{\delta(r - s) \int_0^1 |m(t)|\, \mathrm{d}t + s^{-1} |m(r/s)|\right\} \\ & \times \int_{\Lambda} \mathrm{d}\xi \bigoplus_{n=0}^{\infty} \sum_{j=1}^{n} \sum_{i \in J_j} \chi_{r/2,\xi}(x_j) \chi_{r/2,\xi}(x_i) \\ & + \frac{1}{\epsilon \ln(R/\tilde{a})} \frac{R^2}{s^4} \int_b^{\infty} s^{-1} |m(r/s)| \bigoplus_{n=0}^{\infty} \sum_{j=1}^{n} \sum_{i \in J_j} j\left(\frac{d(x_i, x_j)}{r}\right) \mathrm{d}r \end{aligned} \tag{2.12.16}$$

holds. Here, we have split the integral over r into two parts, one with $s \leq r \leq b$ and one with $b \leq r$. We note that in the second part we do not have the same representation of j as in (2.12.15) as eventually $2r \geq L$. The cutoff parameter b is chosen the same as in the definition of Ω_b^z from (2.10.5).

Let $v_r(\xi)$ denote the integrand of the integral over ξ in (2.12.16). Because $d(x_i, x_k) \geq R/5$ for $i, k \in J_j$, the number of x_i inside a disk of radius $r/2$ is bounded from above by $(1 + 5r/R)^2$. Hence,

$$v_r(\xi) \leq n_{r/2,\xi} \left(1 + \frac{5r}{R}\right)^2 . \tag{2.12.17}$$

On the other hand, we trivially have

$$v_r(\xi) \leq n_{r/2,\xi} \left(n_{r/2,\xi} - 1\right). \tag{2.12.18}$$

Combining these two bounds gives

$$v_r(\xi) \leq f\left(n_{r/2,\xi}\right) \quad \text{where} \quad f(n) = n \min\left\{(n-1), \left(1 + \frac{5r}{R}\right)^2\right\}. \tag{2.12.19}$$

We use the above bounds and $|f(n) - n(1 + \frac{5r}{R})^2| \leq (1 + (1 + \frac{5r}{R})^2)^2/4$ to estimate

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\left[v_r(\xi)\Upsilon_\pi^z\right] &\leq \mathrm{Tr}_{\mathcal{F}}\left[f\left(n_{r/2,\xi}\right)\Upsilon_\pi^z\right] \\ &\leq \mathrm{Tr}_{\mathcal{F}}\left[f\left(n_{r/2,\xi}\right)\Omega_b^z\right] + \left(1 + \frac{5r}{R}\right)^2 \mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right] \\ &\quad + \frac{1}{4}\left(1 + \left(1 + \frac{5r}{R}\right)^2\right)^2 \left\|\Upsilon^z_{\pi,\chi_{r/2,\xi}} - \Omega^z_{b,\chi_{r/2,\xi}}\right\|_1 . \end{aligned} \tag{2.12.20}$$

When integrated over ξ, the second and the third term on the right-hand side of (2.12.20) can be estimated as in (2.11.16) and (2.11.17), respectively. Using a similar estimate as in (2.11.25), we bound the first term from above by

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\left[f\left(n_{r/2,\xi}\right)\Omega_b^z\right] &\leq \min\left\{\mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\left(n_{r/2,\xi} - 1\right)\Omega_b^z\right], \left(1 + \frac{5r}{R}\right)^2 \mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\Omega_b^z\right]\right\} \\ &\leq \min\left\{2\left(\mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\Omega_b^z\right]\right)^2, \left(1 + \frac{5r}{R}\right)^2 \mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\Omega_b^z\right]\right\} \\ &\leq \frac{4\left(\mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\Omega_b^z\right]\right)^2}{1 + 2\,\mathrm{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\Omega_b^z\right]/(1 + 5r/R)^2}. \end{aligned} \tag{2.12.21}$$

Moreover,

$$\operatorname{Tr}_{\mathcal{F}}\left[n_{r/2,\xi}\Omega_b^z\right] = \frac{\pi r^2}{4}\rho_\omega + \langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle. \tag{2.12.22}$$

Using convexity of the function $x \mapsto x^2/(1+x)$, we obtain

$$\operatorname{Tr}_{\mathcal{F}}\left[f\left(n_{r/2,\xi}\right)\Omega_b^z\right] \leq \frac{1}{2}\left(\pi r^2 \rho_\omega\right)^2 + \frac{8\langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle^2}{1 + 4\langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle / (1+5r/R)^2}. \tag{2.12.23}$$

Putting these considerations together and using the assumption $R \leq s \leq r \leq b$, we find

$$\begin{aligned}\int_\Lambda \operatorname{Tr}_{\mathcal{F}}\left[v_r(\xi)\Upsilon_\pi^z\right] \mathrm{d}\xi \leq{}& \frac{|\Lambda|}{2}\left(\pi r^2\rho_\omega\right)^2 + \int_\Lambda \frac{8\langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle^2}{1 + 4\langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle / (1+5r/R)^2}\, \mathrm{d}\xi \\ &+ \frac{9\pi r^4}{R^2}\operatorname{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right] + \frac{b|\Lambda|^{1/2}}{\sqrt{2}} 37^2 \left(\frac{r}{R}\right)^4 S\left(\Upsilon_\pi^z, \Omega_b^z\right)^{1/2}.\end{aligned} \tag{2.12.24}$$

This is the equivalent of [70, Eq. (2.10.20)].

In order to be able to compare the second term on the right-hand side of the above inequality to the last term in (2.11.33), we use the pointwise bound

$$\chi_{r/2,\xi}(x) \leq \frac{(1+5r/R)^2}{\pi(r/2+R/10)^2}\int_{|a|\leq r/2+R/10} \chi_{R/10,\xi+a}(x)\, \mathrm{d}a. \tag{2.12.25}$$

We first use the monotonicity of the map $x \mapsto x^2/(1+x)$ to replace $\chi_{r/2,\xi}(x)$ by the right-hand side of the above equation in the second term on the right-hand side of (2.12.24). Afterwards we use the convexity of the same map and Jensen's inequality to see that

$$\begin{aligned}&\frac{8\langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle^2}{1 + 4\langle \Phi_z | \chi_{r/2,\xi} | \Phi_z \rangle / (1+5r/R)^2} \\ &\quad\leq \frac{(1+5r/R)^4}{\pi(r/2+R/10)^2}\int_{|a|\leq r/2+R/10} \frac{8\langle \Phi_z | \chi_{R/10,\xi+a} | \Phi_z \rangle^2}{1 + 4\langle \Phi_z | \chi_{R/10,\xi+a} | \Phi_z \rangle}\, \mathrm{d}a\end{aligned} \tag{2.12.26}$$

holds. Now we integrate in ξ over Λ and obtain

$$\begin{aligned}&\frac{(1+5r/R)^4}{\pi(r/2+R/10)^2}\int_\Lambda\int_{|a|\leq r/2+R/10} \frac{8\left\langle \Phi_z | \chi_{R/10,\xi+a} | \Phi_z \right\rangle^2}{1 + 4\left\langle \Phi_z | \chi_{R/10,\xi+a} | \Phi_z \right\rangle}\, \mathrm{d}a\, \mathrm{d}\xi \\ &= (1+5r/R)^4 \int_\Lambda \frac{8\langle \Phi_z | \chi_{R/10,\xi} | \Phi_z \rangle^2}{1 + 4\langle \Phi_z | \chi_{R/10,\xi} | \Phi_z \rangle}\, \mathrm{d}\xi \leq (6r/R)^4 \int_\Lambda \frac{8\langle \Phi_z | \chi_{R/10,\xi} | \Phi_z \rangle^2}{1 + \langle \Phi_z | \chi_{R/10,\xi} | \Phi_z \rangle}\, \mathrm{d}\xi.\end{aligned} \tag{2.12.27}$$

The integral in the first term on the right-hand side of (2.12.16) is therefore bounded from above by

$$\begin{aligned}\int_s^b \left\{\delta(r-s)\int_0^1 |m(t)|\,\mathrm{d}t + s^{-1}|m(r/s)|\right\}\int_\Lambda \mathrm{Tr}_{\mathcal{F}}\left[v_r(\xi)\Upsilon_\pi^z\right]\,\mathrm{d}\xi\,\mathrm{d}r \\ \le c\Bigg[\frac{\pi}{4}s^2\left(\frac{6s}{R}\right)^2 \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right] + \frac{b|\Lambda|^{1/2}}{\sqrt{2}}37^2\left(\frac{s}{R}\right)^4 S\left(\Upsilon_\pi^z, \Omega_b^z\right)^{1/2} \\ + \left(\frac{6s}{R}\right)^4 \int_\Lambda \frac{8\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle^2}{1+\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}\,\mathrm{d}\xi + \frac{|\Lambda|}{2}\left(\pi s^2\rho_\omega\right)^2\Bigg],\end{aligned} \tag{2.12.28}$$

where

$$c = \int_0^1 |m(t)|\,\mathrm{d}t + \int_1^\infty |m(t)|t^4\,\mathrm{d}t. \tag{2.12.29}$$

It remains to bound the second term on the right-hand side of (2.12.16) where $r \ge b$. We use (2.9.2) and the same argument that led to (2.12.17) to see that

$$\sum_{i\in J_j} j\left(\frac{d(x_i,x_j)}{r}\right) \le 8\left(1+\frac{5r}{R}\right)^2. \tag{2.12.30}$$

This implies

$$\int_b^\infty s^{-1}|m(r/s)| \bigoplus_{n=0}^\infty \sum_{j=1}^n \sum_{i\in J_j} j\left(\frac{d(x_i,x_j)}{r}\right)\mathrm{d}r \le \mathbb{N}\left(\frac{6s}{R}\right)^2 8\int_{b/s}^\infty |m(r)|r^2\,\mathrm{d}r. \tag{2.12.31}$$

In the following we denote

$$J(b/s) = \int_{b/s}^\infty |m(r)|r^2\,\mathrm{d}r. \tag{2.12.32}$$

Since $|m|$ decays faster than any power, the same holds true for J. The contribution to $\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}_2\Upsilon_\pi^z\right]$ from this part (again except for the prefactor) is therefore bounded from above by

$$\left(\frac{6s}{R}\right)^2 8J(b/s)\left\{\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right] + \mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\Omega_b^z\right]\right\}. \tag{2.12.33}$$

Eqs. (2.12.16), (2.12.28) and (2.12.33) together show that

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}_2\Upsilon_\pi^z\right] \leq \frac{32R^2}{\epsilon\pi s^2\ln(R/\tilde{a})}\Bigg\{&\frac{9\pi\,\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z-\Omega_b^z\right)\right]}{R^2}(c+J(b/s)) \\ &+\frac{9\pi\,\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\Omega_b^z\right]}{R^2}J(b/s)+\frac{37^2cb}{\sqrt{2}R^4}|\Lambda|^{1/2}S(\Upsilon_\pi^z,\Omega_b^z)^{1/2}+\frac{|\Lambda|c\pi^2\rho_\omega^2}{2} \\ &+\left(\frac{6}{R}\right)^4 8c\int_\Lambda\frac{\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle^2}{1+\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}\,\mathrm{d}\xi\Bigg\}\end{aligned} \tag{2.12.34}$$

holds. This is the equivalent[4] of [70, Eq. (2.10.27)].

2.13 Interaction energy, part III

In this section we will put the bounds of the previous two sections together in order to obtain the final lower bound on $\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{W}\Upsilon_\pi^z\right]$. To do so we will distinguish two cases depending on the value of a certain function of Φ_z.

Assume first that

$$\int_\Lambda\frac{\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle^2}{1+\langle\Phi_z|\chi_{R/10,\xi}|\Phi_z\rangle}\,\mathrm{d}\xi \geq \frac{\pi^2}{8}|\Lambda|\left(R^2\rho\right)^2 \tag{2.13.1}$$

holds. Essentially, this conditions means that Φ_z is far from being a constant. In this case, we choose $\lambda = 0$ in (2.11.33). Using the condition (2.13.1), we check that the difference of the last term in (2.11.33) and the last term in (2.12.34) are bounded from below by

$$\frac{4\pi|\Lambda|\rho^2}{\ln(R/a')}\left\{1-\pi\left(\frac{R}{10}\right)^2\rho_\omega-8c\frac{6^4R^2\ln(R/a')}{\epsilon s^2\ln(R/\tilde{a})}\right\}. \tag{2.13.2}$$

Here we used that for our choice of parameters the term in parentheses will be positive (in fact, close to 1).

Next we consider the case when (2.13.1) does not hold, in which case we choose $\lambda = 1$ in (2.11.33). We start by proving some bounds that will turn out to be helpful below. Using (2.12.25) with the choice $r = 3R$ and the monotonicity as well as the convexity of the map $x \mapsto x^2/(1+x)$, we see that

$$\int_\Lambda\frac{\langle\Phi_z|\chi_{3R/2,\xi}|\Phi_z\rangle^2}{1+16^{-2}\langle\Phi_z|\chi_{3R/2,\xi}|\Phi_z\rangle}\,\mathrm{d}\xi \leq 16^4\frac{\pi^2}{8}|\Lambda|\left(R^2\rho\right)^2 \tag{2.13.3}$$

[4] We note that in [70, Eq. (2.10.27)] the first factor $J(b/s)$ on the right side is missing. This is of no consequence, however, as $J(b/s)$ is small for $s \ll b$.

holds in this case. Pick some $D > 0$ and let $\mathcal{B} \subset \Lambda$ be the set

$$\mathcal{B} = \left\{ \xi \in \Lambda \,\middle|\, \langle \Phi_z | \chi_{3R/2,\xi} | \Phi_z \rangle \geq 16^2 D R^2 \rho \right\}. \tag{2.13.4}$$

Using (2.13.3) as well as monotonicity of the map $x \mapsto x/(1+x)$, we obtain

$$\int_{\mathcal{B}} \langle \Phi_z | \chi_{3R/2,\xi} | \Phi_z \rangle \, \mathrm{d}\xi \leq 32\pi^2 |\Lambda| R^2 \rho \left(\frac{1}{D} + R^2 \rho \right). \tag{2.13.5}$$

We proceed similarly to find an estimate for the volume of $\mathcal{B}$:

$$|\mathcal{B}| \leq \frac{\pi^2 |\Lambda|}{8 D^2} \left(1 + D R^2 \rho \right). \tag{2.13.6}$$

We choose $\lambda = 1$ in (2.11.33) and estimate the relevant term from below by

$$\begin{aligned} &\int_{\Lambda} \left[\left(\mathrm{Tr}_{\mathcal{F}} \left[n_{R/2,\xi} \left(n_{R/2,\xi} - 1 \right) \Omega_b^z \right] \right) - 6 \left(\mathrm{Tr}_{\mathcal{F}} \left[n_{3R/2,\xi} \Omega_b^z \right] \right)^3 \right]_+ \mathrm{d}\xi \qquad (2.13.7) \\ &\quad \geq \int_{\Lambda \setminus \mathcal{B}} \left(\left(\mathrm{Tr}_{\mathcal{F}} \left[n_{R/2,\xi} \left(n_{R/2,\xi} - 1 \right) \Omega_b^z \right] \right) - 6 \left(\mathrm{Tr}_{\mathcal{F}} \left[n_{3R/2,\xi} \Omega_b^z \right] \right)^3 \right) \mathrm{d}\xi. \end{aligned}$$

Recall that we defined $\Omega_b^z = U(z) \Omega_b U(z)^\dagger$, where $U(z)$ is the Weyl operator from (2.5.1) and Ω_b is the quasi-free state with one-particle density matrix ω_b defined in (2.10.4). In order to derive a bound on the second term on the right-hand side, we note that $\mathrm{Tr}_{\mathcal{F}} \left[n_{3R/2,\xi} \Omega_b^z \right] = \pi (3R/2)^2 \rho_\omega + \langle \Phi_z | \chi_{3R/2,\xi} | \Phi_z \rangle$. Together with the convexity of the map $x \mapsto x^3$ and (2.13.4) we conclude that

$$\begin{aligned} \int_{\Lambda \setminus \mathcal{B}} \left(\mathrm{Tr}_{\mathcal{F}} \left[n_{3R/2,\xi} \Omega_b^z \right] \right)^3 \mathrm{d}\xi &\leq 4 |\Lambda| \left(\pi (3R/2)^2 \rho_\omega \right)^3 + 4 \int_{\Lambda \setminus \mathcal{B}} \langle \Phi_z | \chi_{3R/2,\xi} | \Phi_z \rangle^3 \, \mathrm{d}\xi \\ &\leq 4 |\Lambda| \left(\pi (3R/2)^2 \rho_\omega \right)^3 + \left(16^2 D R^2 \rho \right)^2 9 \pi R^2 |z|^2 \qquad (2.13.8) \end{aligned}$$

holds.

Now we investigate the first term on the right-hand side of (2.13.7). As in the computation that led to (2.11.25), we write

$$n_{R/2,\xi} \left(n_{R/2,\xi} - 1 \right) = \int_{B_{R/2}(\xi)^2} a_x^\dagger a_y^\dagger a_y a_x \, \mathrm{d}(x,y) \tag{2.13.9}$$

which implies

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}} \left[n_{R/2,\xi} \left(n_{R/2,\xi} - 1 \right) \Omega_b^z \right] &= \mathrm{Tr}_{\mathcal{F}} \left[n_{R/2,\xi} \left(n_{R/2,\xi} - 1 \right) \Omega_b \right] \qquad (2.13.10) \\ &\quad + 2 \langle \Phi_z | \chi_{R/2,\xi} \omega_b \chi_{R/2,\xi} | \Phi_z \rangle + \frac{\pi}{2} R^2 \rho_\omega \langle \Phi_z | \chi_{R/2,\xi} | \Phi_z \rangle + \langle \Phi_z | \chi_{R/2,\xi} | \Phi_z \rangle^2. \end{aligned}$$

Note that we have used the translation invariance of the state Ω_b. Since Ω_b is quasi-free the first term on the right-hand side can be expressed in terms of the one-particle density matrix ω_b. It reads

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}}\left[n_{R/2,\xi}\left(n_{R/2,\xi}-1\right)\Omega_b\right] &= \left(\mathrm{tr}\left[\chi_{R/2,\xi}\omega_b\right]\right)^2 + \mathrm{tr}\left[\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}\omega_b\right] \\ &= (\pi R^2\rho_\omega/4)^2 + \mathrm{tr}\left[\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}\omega_b\right].\end{aligned} \tag{2.13.11}$$

In order to quantify how much the integral of the first term on the right-hand side of (2.13.7) differs from the one with $\Lambda\backslash\mathcal{B}$ replaced by Λ, we estimate

$$\int_{\mathcal{B}} \mathrm{Tr}_{\mathcal{F}}\left[n_{R/2,\xi}\left(n_{R/2,\xi}-1\right)\Omega_b\right] \mathrm{d}\xi \leq 2|\mathcal{B}|(\pi R^2\rho_\omega/4)^2. \tag{2.13.12}$$

To arrive at the right-hand side, we used that the second term in the second line of (2.13.11) is bounded from above by the first one. Since $\langle\Phi_z|\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}|\Phi_z\rangle \leq \mathrm{tr}\,\chi_{R/2,\xi}\omega_b\langle\Phi_z|\chi_{R/2,\xi}|\Phi_z\rangle$, we also have

$$\begin{aligned}&\int_{\mathcal{B}}\left(2\langle\Phi_z|\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}|\Phi_z\rangle + \frac{\pi}{2}R^2\rho_\omega\langle\Phi_z|\chi_{R/2,\xi}|\Phi_z\rangle\right)\mathrm{d}\xi \\ &\leq \pi R^2\rho_\omega\int_{\mathcal{B}}\langle\Phi_z|\chi_{R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi \\ &\leq \pi R^2\rho_\omega 32\pi^2|\Lambda|R^2\rho\left(\frac{1}{D}+R^2\rho\right).\end{aligned} \tag{2.13.13}$$

For the last inequality, we used (2.13.5) and the fact that $\int_{\mathcal{B}}\langle\Phi_z|\chi_{R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi$ is bounded from above by $\int_{\mathcal{B}}\langle\Phi_z|\chi_{3R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi$. For the last term in (2.13.10) we use Schwarz's inequality and (2.13.5) to estimate

$$\begin{aligned}\int_{\Lambda\backslash\mathcal{B}}\langle\Phi_z|\chi_{R/2,\xi}|\Phi_z\rangle^2\,\mathrm{d}\xi &\geq \frac{1}{|\Lambda|}\left(\int_{\Lambda\backslash\mathcal{B}}\langle\Phi_z|\chi_{R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi\right)^2 \\ &\geq |\Lambda|\frac{\pi^2}{16}R^4\left[\rho_z^2 - \pi\rho_z\rho\frac{16^2}{D}\left(1+DR^2\rho\right)\right].\end{aligned} \tag{2.13.14}$$

Here we have again used the notation $\rho_z = |z|^2/|\Lambda|$. Putting all these estimates together, we have the lower bound

$$\int_{\Lambda\setminus\mathcal{B}} \mathrm{Tr}_{\mathcal{F}}\left[n_{R/2,\xi}\left(n_{R/2,\xi}-1\right)\Omega_b^z\right]\mathrm{d}\xi \geq \frac{|\Lambda|\pi^2R^4\rho_\omega^2}{16}\left(1-\frac{\pi^2}{4D^2}\left(1+DR^2\rho\right)\right)$$
$$+\int_\Lambda \mathrm{tr}\left[\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}\omega_b\right]\mathrm{d}\xi + 2\int_\Lambda \langle\Phi_z|\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi$$
$$+|\Lambda|\frac{\pi^2}{16}R^4\left[2\rho_z\rho_\omega+\rho_z^2-\pi\rho_z\rho\frac{16^2}{D}\left(1+DR^2\rho\right)\right]-32|\Lambda|\pi^3R^4\rho_\omega\rho\left(\frac{1}{D}+R^2\rho\right). \tag{2.13.15}$$

We denote $\omega_b(x)=\omega_b(x,0)=\omega_\pi(x,0)\eta_b\left(d(x,0)\right)$. The first term in the second line of (2.13.15) can be written as

$$\int_{\Lambda^3}\chi_{R/2,\xi}(x)\chi_{R/2,\xi}(y)|\omega_b(x,y)|^2\mathrm{d}(x,y,\xi)=\int_{\Lambda^3}\chi_{R/2,\xi}(x+y)\chi_{R/2,\xi}(y)|\omega_b(x)|^2\,\mathrm{d}(x,y,\xi)$$
$$=\frac{|\Lambda|\pi R^2}{32}\int_\Lambda j(d(x,0)/R)|\omega_b(x)|^2\,\mathrm{d}x. \tag{2.13.16}$$

An application of the Cauchy-Schwarz inequality implies

$$\frac{|\Lambda|\pi R^2}{32}\int_\Lambda j(d(x,0)/R)|\omega_b(x)|^2\,\mathrm{d}x \geq \frac{|\Lambda|\pi^2R^4}{16}\gamma_b^2, \tag{2.13.17}$$

where we defined

$$\gamma_b=\frac{1}{2\pi R^2}\int_\Lambda \omega_b(x)j(d(x,0)/R)\,\mathrm{d}x. \tag{2.13.18}$$

We note that $\gamma_b\sim\rho_\omega$ for $b\gg R$ and $\beta^{1/2}\gg R$ and we will give more precise estimates below (see (2.13.29)). It remains to give a lower bound on the second term in the second line of (2.13.15). We claim that

$$\int_\Lambda \langle\Phi_z|\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi \geq |z|^2\frac{\pi^2R^4}{16}\left(\gamma_b-\rho_\omega p_cR\right). \tag{2.13.19}$$

To see this, we write

$$\frac{32}{\pi R^2}\int_\Lambda\langle\Phi_z|\chi_{R/2,\xi}\omega_b\chi_{R/2,\xi}|\Phi_z\rangle\,\mathrm{d}\xi-|z|^2\int_\Lambda\omega_b(x)j\left(\frac{d(x,0)}{R}\right)\mathrm{d}x$$
$$=\int_{\Lambda\times\Lambda}\left(\Phi_z^\dagger(x+y)-\Phi_z^\dagger(y)\right)\Phi_z(y)\omega_b(x)j\left(\frac{d(x,0)}{R}\right)\mathrm{d}(x,y)$$
$$\geq-\|\Phi_z\|_2\int_\Lambda\|\Phi_z(x+\cdot)-\Phi_z(\cdot)\|_2\,|\omega_b(x)|j\left(\frac{d(x,0)}{R}\right)\mathrm{d}x. \tag{2.13.20}$$

We estimate $|\omega_b(x)| \leq \omega_b(0) = \rho_\omega$. Moreover, writing the 2-norm in momentum space one easily checks that $\|\Phi_z(x+\cdot) - \Phi_z(\cdot)\|_2 \leq \|\Phi_z\|_2\, p_c d(x,0)$. Since the support of $j(\cdot/R)$ is the interval $[0,R]$, the integral over Λ can be estimated as

$$\int_\Lambda j(d(x,0)/R) d(x,0)\, \mathrm{d}x \leq 2\pi R^3. \tag{2.13.21}$$

This proves (2.13.19). Combining these estimates with (2.13.8) and (2.13.15) we see that

$$\begin{aligned} &\frac{32}{\pi \ln(R/a')R^4} \int_\Lambda \left[\left(\mathrm{Tr}_{\mathcal{F}} \left[n_{R/2,\xi} \left(n_{R/2,\xi} - 1 \right) \Omega_b^z \right] \right) - 6 \left(\mathrm{Tr}_{\mathcal{F}} \left[n_{3R/2,\xi} \Omega_b^z \right] \right)^3 \right]_+ \mathrm{d}\xi \\ &\geq \frac{2\pi|\Lambda|\rho_\omega^2}{\ln(R/a')} \left(1 - \frac{\pi^2}{4D^2} \left(1 + DR^2\rho \right) \right) + \frac{2\pi|\Lambda|\gamma_b^2}{\ln(R/a')} + \frac{4\pi|\Lambda|\rho_z}{\ln(R/a')} \left(\gamma_b - \rho_\omega p_c R \right) \\ &\quad + \frac{2\pi|\Lambda|}{\ln(R/a')} \left[2\rho_z\rho_\omega + \rho_z^2 - \pi\rho_z\rho \frac{16^2}{D} \left(1 + DR^2\rho \right) \right] - \frac{12 \cdot 3^6 \pi^2 |\Lambda| \rho_\omega^3 R^2}{\ln(R/a')} \\ &\quad - \frac{32^2\pi^2|\Lambda|\rho_\omega\rho}{\ln(R/a')} \left(\frac{1}{D} + R^2\rho \right) - \frac{1728 \cdot 16^4 |\Lambda| (DR^2\rho)^2 \rho_z}{\ln(R/a')R^2}. \end{aligned} \tag{2.13.22}$$

Now we put together the results of this subsection and the two previous ones. More precisely, we combine the estimates from Eqs. (2.11.33), (2.12.34), (2.13.2) and (2.13.22) to obtain

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}} \left[\mathbb{W} \Upsilon_\pi^z \right] \geq{}& \mathrm{Tr}_{\mathcal{F}} \left[\mathbb{N} \left(\Upsilon_\pi^z - \Omega_b^z \right) \right] \left\{ \frac{8}{25 \ln(R/a')R^2} - \frac{288}{\epsilon \ln(R/\tilde{a})s^2} \left(c + J(b/s) \right) \right\} \\ &- \frac{\sqrt{2}}{\pi \ln(R/\tilde{a})R^4} \left(b^2 |\Lambda| S\left(\Upsilon_\pi^z, \Omega_b^z \right) \right)^{1/2} \left\{ 128 + \frac{16 \cdot 37^2 c R^2}{\epsilon s^2} \right\} \\ &- \frac{2\pi|\Lambda|}{\ln(R/\tilde{a})} \left(\frac{144 \left(\rho_\omega + \rho_z \right)}{\pi \epsilon s^2} J(b/s) + \frac{8c\rho_\omega^2 R^2}{\epsilon s^2} \right) + \frac{2\pi|\Lambda|}{\ln(R/a')} \min\{\mathcal{A}_1, \mathcal{A}_2\}. \end{aligned} \tag{2.13.23}$$

To arrive at this result we have used that $a' \leq \tilde{a}$, and we defined

$$\mathcal{A}_1 = 2\rho^2 \left(1 - \pi \left(\frac{R}{10} \right)^2 \rho_\omega - 8c \frac{6^4 R^2 \ln(R/a')}{\epsilon s^2 \ln(R/\tilde{a})} \right) \tag{2.13.24}$$

and

$$\begin{aligned} \mathcal{A}_2 ={}& \rho_\omega^2 + \gamma_b^2 + 2\rho_z\gamma_b + 2\rho_z\rho_\omega + \rho_z^2 \\ &- \rho_\omega^2 \left[\frac{\pi^2}{4D^2} \left(1 + DR^2\rho \right) + 6 \cdot 3^6 \pi \rho_\omega R^2 \right] - 2\rho_z\rho_\omega p_c R - 2\rho_\omega\rho \frac{16^2\pi}{D} \left(1 + DR^2\rho \right) \\ &- \rho\rho_z \left[\frac{864}{\pi} \cdot 16^4 D^2 R^2 \rho + \pi \frac{16^2}{D} \left(1 + DR^2\rho \right) \right] - 16c \frac{6^4 R^2 \rho^2 \ln(R/a')}{\epsilon s^2 \ln(R/\tilde{a})}. \end{aligned} \tag{2.13.25}$$

Below we will choose the parameters such that $\ln(R/\tilde{a})$ and $\ln(R/a')$ are equal to leading order in the dilute limit. We will also choose $\epsilon s^2/R^2$ large enough such that the factor multiplying $\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\left(\Upsilon_\pi^z - \Omega_b^z\right)\right]$ in (2.13.23) is positive. Hence, it will be sufficient to give a lower bound on the difference of the expected particle numbers of Υ_π^z and Ω_b^z, which will be done in the next section.

To simplify the expressions, we make a choice of the parameters ϵ and D and restrict the range of R. We claim that all the terms with a negative sign appearing in $\mathcal{A}_1$ and $\mathcal{A}_2$ (together with the prefactor) can be bounded from below by

$$-\text{const.}\frac{|\Lambda|\rho^2}{|\ln a^2\rho|}\left((R^2\rho)^{1/3} + \frac{R}{s} + p_c R\right). \tag{2.13.26}$$

To see this we employ the bound on ρ_z derived in (2.6.7) as well as the following bound on ρ_ω. Recall that $\ell(p)$ was defined in (2.10.2) and satisfies $\ell(p) \geq \beta(p^2 - \mu_0)$ for all p. This implies

$$\rho_\omega = \frac{1}{|\Lambda|}\sum_p \frac{1}{\mathrm{e}^{\ell(p)} - 1} \leq \frac{1}{|\Lambda|}\sum_p \frac{1}{\mathrm{e}^{\beta(p^2-\mu_0)} - 1} = \rho + o(1) \tag{2.13.27}$$

in the thermodynamic limit. In order to minimize the error terms in $\mathcal{A}_2$, we choose $D = (R^2\rho)^{-1/3}$. On the other hand, note that in the definition of $1/\ln(R/a')$ in (2.9.19) there is a factor $1-\epsilon$, which means there is competition between ϵ and $R^2/(\epsilon s^2)$ to leading order and thus the optimal choice is $\epsilon = R/s$. We also use that $a' \leq \tilde{a} \leq a$ and make the assumption

$$\frac{1}{\ln(R/a)} \lesssim \frac{1}{|\ln a^2\rho|}. \tag{2.13.28}$$

In combination, these considerations prove the claim. Now we give upper and lower bounds on γ_b in terms of ρ_ω as promised above. We claim that

$$\rho_\omega \geq \gamma_b \geq \rho_\omega\left(1 - \frac{\text{const. } R^2}{b^2}\right) - \frac{\text{const. } R^2}{\beta^2} - o(1), \tag{2.13.29}$$

where the $o(1)$ contribution vanishes in the thermodynamic limit. The upper bound can be obtained by noting that $|\omega_b(x)| \leq \omega_b(0) = \rho_\omega$. For the lower bound, recall that $\omega_b(x) = \omega_\pi(x,0)\eta_b(d(x,0))$. We use $\cos(x) \geq 1 - \frac{1}{2}x^2$ to estimate

$$\omega_\pi(x) = \frac{1}{|\Lambda|}\sum_p \frac{\cos(px)}{\mathrm{e}^{\ell(p)} - 1} \geq \rho_\omega - \frac{d(x,0)^2}{2|\Lambda|}\sum_p \frac{p^2}{\mathrm{e}^{\ell(p)} - 1}. \tag{2.13.30}$$

We further use that $|\eta| \leq 1$ and $\eta(t) \geq 1 - \text{const. } t^2$. The support of j being contained in a disk of radius one, we can estimate $d(x,0) \leq R$ inside the integral in (2.13.18). Additionally, we use $\ell(p) \geq \beta p^2$. In combination, the above facts allow us to bound

$$\begin{aligned}\gamma_b &\geq \frac{\rho_\omega}{2\pi R^2} \int_\Lambda \eta(d(x,0)/b) j(d(x,0)/R)\, \mathrm{d}x \\ &\quad - \frac{1}{4\pi|\Lambda| R^2} \sum_p \frac{p^2}{\mathrm{e}^{\ell(p)} - 1} \int_\Lambda d(x,0)^2 \eta(d(x,0)/b) j(d(x,0)/R)\, \mathrm{d}x \\ &\geq \frac{\rho_\omega}{2\pi R^2} \left(\int_\Lambda j(d(x,0)/R)\, \mathrm{d}x - \text{const.} \int_\Lambda \frac{d(x,0)^2}{b^2} j(d(x,0)/R)\, \mathrm{d}x \right) \\ &\quad - \frac{1}{8\pi^2 \beta^2} \int_{\mathbb{R}^2} \frac{p^2}{\mathrm{e}^{p^2} - 1}\, \mathrm{d}p \int_\Lambda j(d(x,0)/R)\, \mathrm{d}x - o(1) \\ &= \rho_\omega \left(1 - \text{const.} \frac{R^2}{b^2} \right) - \text{const.} \frac{R^2}{\beta^2} - o(1). \end{aligned} \tag{2.13.31}$$

This proves (2.13.29).

To estimate the terms in $\mathcal{A}_1$ and $\mathcal{A}_2$ with a positive sign, we apply the lower bound from (2.13.29) to γ_b and find

$$\rho_\omega^2 + \gamma_b^2 + 2\rho_z(\gamma_b + \rho_\omega) + \rho_z^2 \geq 2\rho_\omega^2 + 4\rho_z\rho_\omega + \rho_z^2 - \text{const.} \left(\rho^2 \frac{R^2}{b^2} + \rho \frac{R^2}{\beta^2} \right) - o(1). \tag{2.13.32}$$

In combination, our considerations imply

$$\begin{aligned}\frac{2\pi|\Lambda|}{\ln(R/a')} \min\{\mathcal{A}_1, \mathcal{A}_2\} &\geq \frac{2\pi|\Lambda|}{\ln(R/a')} \min\{2\rho^2, \rho_z^2 + 4\rho_z\rho_\omega + 2\rho_\omega^2\} \\ &\quad - \text{const.} \frac{|\Lambda|\rho^2}{|\ln a^2\rho|} \left((R^2\rho)^{1/3} + \frac{R}{s} + p_c R + \frac{R^2}{b^2} + \frac{R^2}{\beta^2 \rho} \right) - o(|\Lambda|). \end{aligned} \tag{2.13.33}$$

Here, we can drop the terms R^2/b^2 and $R^2/(\beta^2\rho)$ as they are dominated by R/s and $(R^2\rho)^{1/3}$, respectively. This follows from the assumptions $b > s > R, \beta\rho \gtrsim 1$ and $R^2\rho \ll 1$. Using Lemma 3 with the choice $\delta = \sqrt{\ln(R/a)/\varphi}$ as well as the definition of a' in (2.9.19), we estimate

$$\frac{1}{\ln(R/a')} \geq \frac{1}{\ln(R/a)} - \text{const.} \frac{1}{\ln(R/a)} \left(\frac{R}{s} + \kappa + \frac{1}{\sqrt{\varphi \ln(R/a)}} - \frac{R_0^2}{R^2} \ln(R/a) \right). \tag{2.13.34}$$

We will choose $R^2\rho \ll 1$ and, in parcitular, $R^2\rho \leq 1$, i.e.,

$$\frac{1}{\ln(R/a)} \geq \frac{2}{|\ln a^2\rho|}. \tag{2.13.35}$$

Note the factor two on the right side which is important to give the correct leading order contribution for the terms with positive sign below. We thus finally arrive at

$$\frac{2\pi|\Lambda|}{\ln(R/a')}\min\{\mathcal{A}_1,\mathcal{A}_2\} \geq \frac{4\pi|\Lambda|}{|\ln a^2\rho|}\min\{2\rho^2,\rho_z^2+4\rho_z\rho_\omega+2\rho_\omega^2\} \\ -\text{const.}\frac{|\Lambda|\rho^2}{|\ln a^2\rho|}\left((R^2\rho)^{1/3}+\frac{R}{s}+p_cR+\kappa+\frac{1}{\sqrt{\varphi|\ln a^2\rho|}}+\frac{R_0^2}{R^2}|\ln a^2\rho|\right). \tag{2.13.36}$$

2.14 A bound on the number of particles

In this section we give a lower bound on the terms involving the number operator and its square. More precisely, we consider the sum of the first term from (2.13.23) and the term $\frac{1}{2}\operatorname{Tr}_{\mathcal{F}}[\mathbb{K}\Upsilon^z]$ from (2.9.30). Recalling that we already chose $\epsilon = R/s$ and that $\mathbb{K}$ was defined in (2.4.3), we seek a lower bound on the expression

$$\mathcal{N} = \left\{\frac{8}{25\ln(R/a')R^2} - \frac{288}{\ln(R/\tilde{a})Rs}(c+J(b/s))\right\}\operatorname{Tr}_{\mathcal{F}}[\mathbb{N}(\Upsilon_\pi^z-\Omega_b^z)] \\ +\frac{2\pi C}{|\Lambda||\ln a^2\rho|}\operatorname{Tr}_{\mathcal{F}}[(\mathbb{N}-N)^2\Upsilon^z]. \tag{2.14.1}$$

The fact that we need to give a bound for the first term on the right-hand side is one of the reasons for introducing the operator $\mathbb{K}$ in Section 2.4.

Using the definition of Ω_b and Ω_π in (2.10.3)–(2.10.5) and the fact that they have the same density, we conclude

$$\operatorname{Tr}_{\mathcal{F}}[\mathbb{N}(\Upsilon_\pi^z-\Omega_b^z)] = \operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z-\Gamma_0)], \tag{2.14.2}$$

where

$$\mathcal{N}^> = \sum_{|p|\geq p_c} a_p^\dagger a_p. \tag{2.14.3}$$

For the quadratic term, we use the inequality

$$(\mathbb{N}-N)^2 \geq (|z|^2+\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0]-N)^2+2(|z|^2+\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0]-N)(\mathbb{N}-|z|^2-\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0]). \tag{2.14.4}$$

This implies

$$\operatorname{Tr}_{\mathcal{F}}[(\mathbb{N}-N)^2\Upsilon^z] \geq (|z|^2+\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0]-N)^2 \\ +2(|z|^2+\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0]-N)\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z-\Gamma_0)]. \tag{2.14.5}$$

Hence, we obtain the following expression as a lower bound

$$\begin{aligned}\mathcal{N} \geq\ & \frac{2\pi C}{|\Lambda| |\ln a^2\rho|}(|z|^2 + \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0] - N)^2 \\ & + \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z - \Gamma_0)]\Bigg[\left\{\frac{8}{25\ln(R/a')R^2} - \frac{288}{\ln(R/\tilde{a})Rs}(c + J(b/s))\right\} \\ & + \frac{4\pi C}{|\Lambda| |\ln a^2\rho|}(|z|^2 + \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0] - N)\Bigg]. \end{aligned} \tag{2.14.6}$$

We will choose the parameters R, s and C satisfying the conditions $C \ll 1/(R^2\rho)$ and $R \ll s$ such that the term in square brackets on the right-hand side of (2.14.6) is always positive (for any value of $|z|$) and therefore we need a lower bound on the expression $\mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z - \Gamma_0)]$.

Let

$$\tilde{f}(\mu) = \frac{1}{\beta}\sum_{|p|\geq p_c} \ln\left(1 - \mathrm{e}^{-\beta(p^2-\mu_0-\mu)}\right). \tag{2.14.7}$$

By the variational principle for the free energy, we have for any $\mu \leq 0$

$$S(\Gamma^z, \Gamma_0) - \beta\mu\, \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma^z] \geq \beta(\tilde{f}(\mu) - \tilde{f}(0)). \tag{2.14.8}$$

From the absolute monotonicity[5] of $\tilde{f}$ (i.e., all derivatives being negative), we obtain

$$\tilde{f}(\mu) \geq \tilde{f}(0) + \mu\tilde{f}'(0) + \frac{1}{2}\mu^2\tilde{f}''(0). \tag{2.14.9}$$

We have

$$\tilde{f}'(\mu) = -\sum_{|p|\geq p_c} \frac{1}{\mathrm{e}^{\beta(p^2-\mu_0-\mu)} - 1} \tag{2.14.10}$$

and therefore $\tilde{f}'(0) = -\mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0]$. The second derivative of $\tilde{f}$ is given by

$$\tilde{f}''(\mu) = -\frac{\beta}{2}\sum_{|p|\geq p_c} \frac{1}{\cosh(\beta(p^2 - \mu_0 - \mu)) - 1}. \tag{2.14.11}$$

Hence,

$$S(\Gamma^z, \Gamma_0) - \beta\mu\, \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma^z] \geq -\beta\mu\, \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0] - \frac{1}{4}\mu^2\beta^2 \sum_{|p|\geq p_c} \frac{1}{\cosh(\beta(p^2 - \mu_0)) - 1}. \tag{2.14.12}$$

[5]The term *absolute monotonicity* is often used if all derivatives of a function f share the same sign, $f^{(n)} \gtrless 0$. In contrast, the term *complete monotonicity* (or total monotonicity) is often used to indicate that the derivatives switch sign at every order, $(-1)^n f^{(n)} \gtrless 0$.

Since $\mu \leq 0$, this can be rewritten as

$$\mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z - \Gamma_0)] \geq -\frac{1}{\beta|\mu|} S(\Gamma^z, \Gamma_0) - \frac{\beta|\mu|}{4} \sum_{|p|\geq p_\mathrm{c}} \frac{1}{\cosh(\beta(p^2 - \mu_0)) - 1}. \tag{2.14.13}$$

Optimizing the right-hand side over μ, we find

$$\mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z - \Gamma_0)] \geq -\left(S(\Gamma^z, \Gamma_0) \sum_{|p|\geq p_\mathrm{c}} \frac{1}{\cosh(\beta(p^2 - \mu_0)) - 1} \right)^{1/2}. \tag{2.14.14}$$

We can use the a priori bound from (2.6.4) to bound the relative entropy, while for the sum over p we use the bound $\cosh x - 1 \geq x^2/2$. Thus,

$$\sum_{|p|\geq p_\mathrm{c}} \frac{1}{\cosh(\beta(p^2 - \mu_0))} \leq \frac{2}{\beta^2} \sum_{|p|\geq p_\mathrm{c}} \frac{1}{(p^2 - \mu_0)^2} = \frac{|\Lambda|}{2\beta^2\pi^2} \int_{|p|\geq p_\mathrm{c}} \frac{\mathrm{d}p}{(p^2 - \mu_0)^2} + o(|\Lambda|). \tag{2.14.15}$$

The integral equals

$$\int_{|p|\geq p_\mathrm{c}} \frac{\mathrm{d}p}{(p^2 - \mu_0)^2} = \pi \int_{p_\mathrm{c}^2}^{\infty} \frac{\mathrm{d}x}{(x - \mu_0)^2} = \frac{\pi}{p_c^2 - \mu_0}. \tag{2.14.16}$$

In conclusion, we have shown that

$$\mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>(\Gamma^z - \Gamma_0)] \geq -\left(\frac{4|\Lambda|^2\rho^2}{|\ln a^2\rho|(\beta p_c^2 - \beta\mu_0)} \right)^{1/2} - o(|\Lambda|). \tag{2.14.17}$$

We now apply this to (2.14.6) and obtain

$$(2.14.1) = \mathcal{N} \geq \frac{2\pi C}{|\Lambda||\ln a^2\rho|} (|z|^2 + \mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0] - N)^2 - Z^{(3)} - o(|\Lambda|), \tag{2.14.18}$$

where

$$\begin{aligned} Z^{(3)} :=\ &\mathrm{const.} \frac{|\Lambda|\rho^2}{|\ln a^2\rho|^{3/2}(\beta p_\mathrm{c}^2 - \beta\mu_0)^{1/2}} \left[|\ln a^2\rho| \left\{ \frac{8}{25\ln(R/a')R^2\rho} \right.\right. \\ &\left.\left. - \frac{288}{\ln(R/\tilde{a})Rs\rho}(c + J(b/s)) \right\} + 4\pi C \left(\frac{2}{\sqrt{C}} + \frac{\rho_\omega}{\rho} \right) \right]. \end{aligned} \tag{2.14.19}$$

Note that we used (2.6.7) to bound ρ_z as well as $|\Lambda|^{-1}\,\mathrm{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0] \leq \rho_\omega$. Using also (2.13.27), the assumption (2.13.28) on R and choosing $C \ll 1/(R^2\rho)$, this simplifies to

$$Z^{(3)} \lesssim \frac{|\Lambda|\rho^2}{|\ln a^2\rho|} \frac{1}{(|\ln a^2\rho|(\beta p_\mathrm{c}^2 - \beta\mu_0))^{1/2} R^2\rho}. \tag{2.14.20}$$

2.15 Relative entropy, effect of cutoff

In this section we quantify the effect of the cutoff parameter b on the relative entropy $S(\Upsilon^z_\pi, \Omega^z_b)$ appearing in (2.13.23). The goal is to estimate $S(\Upsilon^z_\pi, \Omega^z_b)$ in terms of $S(\Pi \otimes \Gamma^z, \Omega_\pi) = S(\Gamma^z, \Gamma_0)$. For the latter expression we have the a priori bound (2.6.4). To obtain such an estimate it will be important that the vacuum state Π_0 has been replaced by the more general quasi-free state Π in Section 2.7.

For any quasi-free state Ω_ω with one-particle density matrix ω and any state Γ it is easy to check that the relative entropy $S(\Gamma, \Omega_\omega)$ is convex in ω. The one-particle density matrix of Ω_b is given by the following convex combination

$$\omega_b = \frac{1}{|\Lambda|} \sum_q \hat{\eta}_b(q) \frac{1}{2} \left(\omega_\pi(p+q) + \omega_\pi(p-q) \right) |p\rangle\langle p|. \tag{2.15.1}$$

Convexity of the map $\omega \mapsto S(\Gamma, \Omega_\omega)$ therefore implies

$$S\left(\Pi \otimes \Gamma^z, \Omega_b\right) \leq \frac{1}{|\Lambda|} \sum_q \hat{\eta}_b(q) S\left(\Pi \otimes \Gamma^z, \Omega_q\right), \tag{2.15.2}$$

where Ω_q is the quasi-free state corresponding to the one-particle density matrix with eigenvalues $\frac{1}{2}\left(\omega_\pi(p+q) + \omega_\pi(p-q)\right)$. Further arguments based on convexity (see [68, Eqs. (5.15) and (5.16)]) yield

$$\begin{aligned} S(\Pi \otimes \Gamma^z, \Omega_q) \leq{}& \left(1 + t^{-1}\right) S(\Gamma^z, \Gamma_0) \\ &+ \sum_p \left(h_q(p) - h_0(p)\right) \left(\frac{1}{e^{h_0(p) + t(h_0(p) - h_q(p))} - 1} - \frac{1}{e^{h_q(p)} - 1} \right) \end{aligned} \tag{2.15.3}$$

for any $t > 0$. Here we defined

$$h_q(p) = \ln \left(\frac{2 + \omega_\pi(p+q) + \omega_\pi(p-q)}{\omega_\pi(p+q) + \omega_\pi(p-q)} \right). \tag{2.15.4}$$

To estimate (2.15.3) from above, we require the following lemma. Since the proof of the analogous [70, Lemma 6] does not explicitly depend on the dimension of the configuration space it translates to the two-dimensional case without changes. We therefore omit the proof of Lemma 8.

Lemma 8. *Let $\ell : \mathbb{R}^2 \to \mathbb{R}_+$, and let $L_\pm = \pm \sup_p \sup_{|q|=1} \pm (q\nabla)^2 \ell(p)$ denote the supremum (infimum) of the largest (smallest) eigenvalue of the Hessian of ℓ. Let $\omega_\pi(p) = [e^{\ell(p)} - 1]^{-1}$, and let $h_q(p)$ be given as in* (2.15.4). *Then*

$$h_q(p) - h_0(p) \leq L_+ q^2, \tag{2.15.5}$$

and

$$h_q(p) - h_0(p) \\ \geq q^2 L_- + q^2 \min\{L_-, 0\} - 4q^2 \sup_p [|\nabla \ell(p)|^2 \omega_\pi(p)] - 2q^2(|q| + |p|)^2 \sup_p [|\nabla \ell(p)|^2/p^2]. \tag{2.15.6}$$

Recall that the $\ell(p)$ in question was defined in (2.10.2). Now we choose the parameters π_p which determine $\ell(p)$ for $|p| < p_c$. For that purpose let $g : \mathbb{R}^2 \to [0,1]$ be a smooth radial function that is supported in a disk of radius one and assume that $g(p) \geq \frac{1}{2}$ for $|p| \leq \frac{1}{2}$. Then we set

$$\ell(p) = \beta(p^2 - \mu_0) + \beta p_c^2 g(p/p_c). \tag{2.15.7}$$

This corresponds to the choice

$$\pi_p = \frac{1}{e^{\beta(p^2-\mu_0)+\beta p_c^2 g(p/p_c)} - 1}. \tag{2.15.8}$$

Note that this choice indeed satisfies our earlier assumption on $\ell(p)$, which was $\ell(p) \geq \beta(p^2 - \mu_0)$. Furthermore, we can estimate $\pi_p \lesssim 1/(\beta(p_c^2 - \mu_0))$. This can be seen by considering $|p| \geq p_c/2$ and $|p| < p_c/2$ separately and using $\ell(p) \geq \beta(p^2 - \mu_0)$ in the first case and $g(p/p_c) \geq 1/2$ in the second case. Using this and $M \lesssim p_c^2|\Lambda|$, we can bound P from Section 2.7 as

$$P = \sum_{|p| \leq p_c} \pi_p \lesssim \frac{M}{\beta(p_c^2 - \mu_0)} \lesssim \frac{|\Lambda| p_c^2}{\beta(p_c^2 - \mu_0)}, \tag{2.15.9}$$

The bound on P is needed for estimating the term $Z^{(2)}$ in (2.7.7).

For our choice of ℓ it is easy to see that both L_+/β and L_-/β are bounded independently of all parameters. We further have the bounds $|\nabla \ell(p)| \lesssim \beta|p|$ and $\omega_\pi(p) \leq \ell(p)^{-1} \leq (\beta p^2)^{-1}$, and together with Lemma 8, this implies

$$-B\beta q^2 \left(1 + \beta(|p| + |q|)^2\right) \leq h_q(p) - h_0(p) \leq B\beta q^2 \tag{2.15.10}$$

for some $B > 0$. Using $\sinh(x)/x \leq \cosh(x)$ for $x \in \mathbb{R}$, we estimate

$$\left(h_q(p) - h_0(p)\right)\left(\frac{1}{e^{h_0(p)+t(h_0(p)-h_q(p))} - 1} - \frac{1}{e^{h_q(p)} - 1}\right) \\ \leq \frac{1}{2}(1+t)\left(h_q(p) - h_0(p)\right)^2 \frac{e^{-h_q(p)} + e^{-h_0(p)+t(h_q(p)-h_0(p))}}{\left(1 - e^{-h_0(p)+t(h_q(p)-h_0(p))}\right)\left(1 - e^{-h_q(p)}\right)}. \tag{2.15.11}$$

We use

$$\left(h_q(p) - h_0(p)\right)^2 \leq B^2 \left(\beta q^2\right)^2 \left(1 + \beta\,(|p| + |q|)^2\right)^2 \tag{2.15.12}$$

as well as the fact that the last fraction on the right-hand side of (2.15.11) is bounded from above by

$$\begin{aligned}&\frac{\mathrm{e}^{-h_q(p)} + \mathrm{e}^{-h_0(p)+t\beta B q^2}}{\left(1 - \mathrm{e}^{-h_0(p)+t\beta B q^2}\right)\left(1 - \mathrm{e}^{-h_q(p)}\right)} \\ &= \omega^t(p) + \frac{1}{2}\left(\omega_\pi(p+q) + \omega_\pi(p-q)\right)\left(1 + 2\omega^t(p)\right),\end{aligned} \tag{2.15.13}$$

where $\omega^t(p) = [\mathrm{e}^{h_0(p)-B\beta t q^2} - 1]^{-1}$. To obtain this result, we assumed that t is small enough such that $h_0(p) - B\beta t q^2 > 0$ for all p. Since sums converge to integrals in the thermodynamic limit we need to bound

$$\int_{\mathbb{R}^2} \left(1 + \beta\,(|p| + |q|)^2\right)^2 \left(\omega^t(p) + \frac{1}{2}\left(\omega_\pi(p+q) + \omega_\pi(p-q)\right)\left(1 + 2\omega^t(p)\right)\right) \mathrm{d}p. \tag{2.15.14}$$

We replace $\omega_\pi(p-q)$ by $\omega_\pi(p+q)$ without changing the value of the integral. Then we use $\omega_\pi(p) \leq \omega^t(p)$, change variables $p \to p - q$ and use Schwarz's inequality to see that (2.15.14) is bounded from above by

$$\begin{aligned}(2.15.14) &\leq \int_{\mathbb{R}^2} \left(1 + \beta(|p| + |q|)^2\right)^2 \left(\omega^t(p) + \omega^t(p+q)(1 + 2\omega^t(p))\right) \mathrm{d}p \\ &\leq 2\int_{\mathbb{R}^2} \left(1 + \beta(|p| + 2|q|)^2\right)^2 \omega^t(p)\,\mathrm{d}p \\ &\quad + \left(\int_{\mathbb{R}^2} \left(1 + \beta(|p| + |q|)^2\right)^2 (\omega^t(p+q))^2\,\mathrm{d}p\right)^{1/2} \\ &\quad \times \left(4\int_{\mathbb{R}^2} \left(1 + \beta(|p| + |q|)^2\right)^2 (\omega^t(p))^2\,\mathrm{d}p\right)^{1/2} \\ &\leq 2\int_{\mathbb{R}^2} \left(1 + \beta\,(|p| + 2|q|)^2\right)^2 \omega^t(p)\left(1 + \omega^t(p)\right) \mathrm{d}p.\end{aligned} \tag{2.15.15}$$

We choose $t = \min\{1, (b^2 q^2)^{-1}\}$. We then have $tq^2 \leq b^{-2}$ and further

$$\ell(p) - B\beta t q^2 \geq \beta\left[\frac{p^2}{2} - \mu_0 + p_{\mathrm{c}}^2\left(\frac{1}{8} - \frac{B}{b^2 p_{\mathrm{c}}^2}\right)\right] \geq \beta\left[\frac{p^2}{2} - \mu_0 + \frac{p_c^2}{16}\right], \tag{2.15.16}$$

which can be seen by considering, similarly to before when estimating P in (2.15.9), $|p| \geq p_{\mathrm{c}}/2$ and $|p| < p_{\mathrm{c}}/2$ separately. For the last inequality, we already assumed that b and

p_c will be chosen in such a way that $b^2 p_c^2 \gg 1$ and, in particular, $B/(b^2 p_c^2) \leq 1/16$ holds. Denoting

$$\tau = -\beta\mu_0 + \frac{\beta p_c^2}{16}, \tag{2.15.17}$$

we thus have the bound

$$\omega^t \leq \left(e^{\tau + \beta p^2/2} - 1\right)^{-1} \leq e^{-\tau - \beta p^2/2}\left[1 + \frac{1}{\tau + \beta p^2/2}\right]. \tag{2.15.18}$$

Inserting (2.15.18) into (2.15.15), we find

$$\begin{aligned}
(2.15.15) \leq 2 \int_{\mathbb{R}^2} &\left(1 + \beta(|p| + 2|q|)^2\right)^2 e^{-\tau - \beta p^2/2}\left[1 + \frac{1}{\tau + \beta p^2/2}\right] \\
&\times \left(1 + e^{-\tau - \beta p^2/2}\left[1 + \frac{1}{\tau + \beta p^2/2}\right]\right) dp \\
&\lesssim \frac{e^{-\tau}}{\beta}\left(1 + \beta^2 q^4\right) \int_{\mathbb{R}^2} \left(1 + p^4\right) e^{-p^2/2}\left[1 + \frac{1}{(\tau + p^2/2)^2}\right] dp \\
&\lesssim \frac{e^{-\tau}}{\beta}\left(1 + \beta^2 q^4\right)\left(1 + \tau^{-1}\right).
\end{aligned} \tag{2.15.19}$$

We combine the above equations and use $t^{-1} \leq 1 + b^2 q^2$ to see that

$$S(\Pi \otimes \Gamma^z, \Omega_q) \lesssim \left(2 + b^2 q^2\right) S(\Gamma^z, \Gamma_0) + \frac{|\Lambda|}{\tau}\beta q^4\left(1 + \beta^2 q^4\right) + o(|\Lambda|) \tag{2.15.20}$$

holds. Using (2.15.2) and $\eta_b(0) = 1$, we therefore have

$$S(\Pi \otimes \Gamma^z, \Omega_b) \lesssim S(\Gamma^z, \Gamma_0) + \frac{\beta}{\tau}\sum_q \hat{\eta}_b(q) q^4\left(1 + \beta^2 q^4\right) + o(|\Lambda|). \tag{2.15.21}$$

We will choose b such that $b^2 \gg \beta$ and this implies, in particular, that $\beta b^{-2} \lesssim 1$. We therefore have

$$S(\Pi \otimes \Gamma^z, \Omega_b) \lesssim S(\Gamma^z, \Gamma_0) + \frac{\beta|\Lambda|}{\tau b^4} + o(|\Lambda|). \tag{2.15.22}$$

The above inequality quantifies the effect of the cutoff. From (2.13.23), we know that we still have to multiply the relative entropy term by b^2. Using also the a priori bound from (2.6.4), we obtain

$$\begin{aligned}
b^2 S(\Upsilon_\pi^z, \Omega_b^z) &\lesssim b^2\left(S(\Gamma^z, \Gamma_0) + \frac{\beta|\Lambda|}{\tau b^4} + o(|\Lambda|)\right) \\
&\lesssim \beta|\Lambda|\left(\frac{b^2\rho^2}{|\ln a^2\rho|} + \frac{1}{\tau b^2} + o(1)\right).
\end{aligned} \tag{2.15.23}$$

From this expression it is easy to read off the optimal choice of b which is given (up to a constant factor) by

$$b = \left(\frac{|\ln a^2\rho|}{\tau\rho^2} \right)^{1/4}. \tag{2.15.24}$$

The result of this section is therefore the following bound on the relative entropy

$$b^2 S(\Upsilon_\pi^z, \Omega_b^z) \lesssim |\Lambda| \left(\frac{\beta\rho}{(\tau|\ln a^2\rho|)^{1/2}} + o(1) \right). \tag{2.15.25}$$

2.16 Final lower bound

In this section we collect the above estimates to give a lower bound on $F_z(\beta)$, which in turn will give a lower bound on the free energy. Recall from Sections 2.5 and 2.5 that

$$\begin{aligned} \frac{1}{|\Lambda|} F(\beta, N, |\Lambda|) &= -\frac{1}{\beta|\Lambda|} \ln \operatorname{Tr}_N \mathrm{e}^{-\beta H_N} \geq -\frac{1}{\beta|\Lambda|} \ln \operatorname{Tr}_N \mathrm{e}^{-\beta \tilde{H}_N} \\ &\geq -\frac{1}{\beta|\Lambda|} \operatorname{Tr}_{\mathcal{F}} \mathrm{e}^{-\beta \mathbb{H}} \geq -\frac{1}{\beta|\Lambda|} \ln \int_{\mathbb{C}^M} \operatorname{Tr}_{\mathcal{F}} \mathrm{e}^{-\beta \mathbb{H}^{\mathrm{s}}(z)} \, \mathrm{d}z \\ &\geq \frac{1}{|\Lambda|} \left[\mu_0 N - \frac{1}{\beta} \ln \int_{\mathbb{C}^M} \mathrm{e}^{-\beta F_z(\beta)} \, \mathrm{d}z - Z^{(1)} \right], \end{aligned} \tag{2.16.1}$$

where $Z^{(1)}$ was defined in (2.5.8). Now we combine the estimates from (2.9.30), (2.13.23), (2.13.36) as well as (2.14.18) and (2.15.25) to obtain the final lower bound to $F_z(\beta)$ as

$$\begin{aligned} F_z(\beta) \geq &-\frac{1}{\beta} \ln \operatorname{Tr}_{\mathcal{F}_>} [\mathrm{e}^{-\beta \mathbb{T}_s^c(z)}] - Z^{(2)} - Z^{(3)} - Z^{(4)} - o(|\Lambda|) \\ &+ \frac{2\pi C}{|\Lambda||\ln a^2\rho|} \left(|z|^2 + \operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^> \Gamma_0] - N \right)^2 + \frac{4\pi|\Lambda|}{|\ln a^2\rho|} \min\left\{ \rho_z^2 + 4\rho_z\rho_\omega + 2\rho_\omega^2, 2\rho^2 \right\}. \end{aligned} \tag{2.16.2}$$

Here, the error terms $Z^{(2)}$ and $Z^{(3)}$ are defined in (2.7.7) and (2.14.19), respectively. The error term $Z^{(4)}$ contains the remaining errors and is defined by

$$\begin{aligned} Z^{(4)} := \text{const.} \frac{|\Lambda|\rho^2}{|\ln a^2\rho|} &\left(\frac{1}{R^4\rho^2} \frac{(\beta\rho)^{1/2}}{\tau^{1/4}|\ln a^2\rho|^{1/4}} + \frac{1}{Rs\rho} J\left(\frac{|\ln a^2\rho|^{1/4}}{\tau^{1/4}\rho^{1/2} s} \right) + \frac{R}{s} \right. \\ &\left. + (R^2\rho)^{1/3} + p_c R + \kappa + \frac{1}{\sqrt{\varphi|\ln a^2\rho|}} + \frac{R_0^2}{R^2}|\ln a^2\rho| \right) + \text{const.} \frac{|\Lambda| p_c^2}{\beta} \frac{R_0^2}{R^2}. \end{aligned} \tag{2.16.3}$$

To obtain this form of the error term we also used (2.13.28) to replace the logarithmic factors $\ln(R/a)$ by the desired factor $|\ln a^2\rho|$ and inserted the choices $\epsilon = R/s$ and $b = (|\ln a^2\rho|/(\tau\rho^2))^{1/4}$ made earlier. The last term in $Z^{(4)}$ originates from the term $(\kappa - \kappa')\sum_p p^2\pi_p$ in (2.9.30) using (2.9.21) and (2.15.9).

Let us have a closer look at the two terms in the second line of (2.16.2). We define

$$\rho^0 = \frac{1}{|\Lambda|}\operatorname{Tr}_{\mathcal{F}_>}[\mathbb{N}^>\Gamma_0] = \rho_\omega - \frac{P}{|\Lambda|}, \tag{2.16.4}$$

where $P = \operatorname{tr}\pi = \sum_{|p|<p_c}\pi_p$ was defined in Section 2.7. Using $\rho^0 \leq \rho_\omega$, we replace ρ_ω in the second term in the second line of (2.16.2) by ρ^0 for a lower bound. When we minimize over ρ_z we find

$$\begin{aligned}&\frac{C}{2}\left(\rho_z - (\rho-\rho^0)\right)^2 + \rho_z^2 + 4\rho_z\rho^0 + 2(\rho^0)^2\\ &\geq \frac{1}{1+2/C}\left(2\rho^2 - (\rho-\rho^0)^2 - \frac{4}{C}(\rho^0)^2\right),\end{aligned} \tag{2.16.5}$$

Note that the right-hand side of (2.16.5) is bounded by $2\rho^2$. This implies in particular that the minimum in (2.16.2) will be attained by the first term when we minimize over ρ_z. Therefore, we have the lower bound

$$\begin{aligned}F_z(\beta) \geq& -\frac{1}{\beta}\ln\operatorname{Tr}_{\mathcal{F}_>}\mathrm{e}^{-\beta\mathbb{T}_s^c(z)} - \sum_{i=1}^4 Z^{(i)} - o(|\Lambda|)\\ &+ \frac{4\pi|\Lambda|}{|\ln a^2\rho|}\left(2\rho^2 - (\rho-\rho^0)^2 - \frac{4}{C}\rho^2\right),\end{aligned} \tag{2.16.6}$$

where we used

$$\rho^0 = \frac{1}{4\pi^2}\int_{|p|>p_c}\frac{\mathrm{d}p}{\mathrm{e}^{\beta(p^2-\mu_0)}} + o(1) \leq \rho(1+o(1)) \tag{2.16.7}$$

in the $1/C$ correction term. The only remaining z dependence is then in the first term

$$-\frac{1}{\beta}\ln\operatorname{Tr}_{\mathcal{F}_>}\mathrm{e}^{-\beta\mathbb{T}_s^c(z)} = \sum_{|p|<p_c}\epsilon(p)|z_p|^2 + \frac{1}{\beta}\sum_{|p|\geq p_c}\ln\left(1-\mathrm{e}^{-\beta\epsilon(p)}\right), \tag{2.16.8}$$

where $\epsilon(p)$ was defined in (2.9.25) as $\epsilon(p) = \kappa' p^2 + (1-\kappa)p^2(1-\chi(p)^2) - \mu_0$, with χ a cutoff function at the scale $s \geq R$. We evaluate the integral over $\mathbb{C}^M$ in (2.16.1) to give

$$\int_{\mathbb{C}^M}\mathrm{e}^{-\beta\sum_{|p|<p_c}\epsilon(p)|z_p|^2}\,\mathrm{d}z = \prod_{|p|<p_c}\int_{\mathbb{C}}\mathrm{e}^{-\beta\epsilon(p)|z_p|^2}\,\mathrm{d}z_p = \prod_{|p|<p_c}\frac{1}{\beta\epsilon(p)}. \tag{2.16.9}$$

Now we estimate the term that contributes to the free part of the free energy. Using the fact that $x \geq 1 - \mathrm{e}^{-x}$ for $x \geq 0$, we find

$$\begin{aligned}\frac{1}{\beta|\Lambda|}\sum_{|p|<p_{\mathrm{c}}} \ln(\beta\epsilon(p)) + \frac{1}{\beta|\Lambda|}\sum_{|p|\geq p_{\mathrm{c}}} \ln\left(1-\mathrm{e}^{-\beta\epsilon(p)}\right) \\ \geq \frac{1}{\beta|\Lambda|}\sum_{p} \ln\left(1-\mathrm{e}^{-\beta\epsilon(p)}\right) \geq \frac{1}{4\beta\pi^2}\int_{\mathbb{R}^2} \ln\left(1-\mathrm{e}^{-\beta\epsilon(p)}\right)\mathrm{d}p - o(1).\end{aligned} \tag{2.16.10}$$

We split the integral into two parts $|p| \leq s^{-1}$ and $|p| \geq s^{-1}$. In the first part we have $\epsilon(p) = (1-\kappa+\kappa')p^2 - \mu_0$, while in the second part we have the bound $\epsilon(p) \geq \kappa' p^2$. Hence,

$$\begin{aligned}\int_{\mathbb{R}^2} \ln\left(1-\mathrm{e}^{-\beta\epsilon(p)}\right)\mathrm{d}p \\ \geq \frac{1}{1-\kappa+\kappa'}\int_{\mathbb{R}^2} \ln\left(1-\mathrm{e}^{-\beta(p^2-\mu_0)}\right)\mathrm{d}p + \frac{1}{\kappa'\beta}\int_{|p|^2\geq\kappa'\beta/s^2} \ln\left(1-\mathrm{e}^{-p^2}\right)\mathrm{d}p.\end{aligned} \tag{2.16.11}$$

The parameter s will be chosen such that $s^2 \ll \kappa'\beta$; the second integral is then exponentially small in the parameter $s^2/(\kappa'\beta)$.

Define

$$\rho_{\mathrm{s}} := \rho\left[1 - \frac{\ln|\ln a^2\rho|}{4\pi\beta\rho}\right]_+. \tag{2.16.12}$$

Our goal is to bound $\rho - \rho^0$ by ρ_{s} plus an error term. This will be achieved by introducing a new parameter $\tilde{p}_{\mathrm{c}}$ that satisfies

$$\frac{1}{4\pi^2}\int_{|p|\leq\tilde{p}_{\mathrm{c}}} \frac{\mathrm{d}p}{\mathrm{e}^{\beta(p^2-\mu_0)}-1} = \rho_{\mathrm{s}}. \tag{2.16.13}$$

By an explicit computation, we find

$$\beta\tilde{p}_{\mathrm{c}}^2 = \frac{1}{\mathrm{e}^{4\pi\beta\rho}-1}\left[\frac{\mathrm{e}^{4\pi\beta\rho}}{|\ln a^2\rho|} - 1\right]_+. \tag{2.16.14}$$

We remark that p_{c} will be chosen such that $p_{\mathrm{c}} \geq \tilde{p}_{\mathrm{c}}$ holds, and we use (2.16.7) to write

$$\rho - \rho^0 = \rho_{\mathrm{s}} + \frac{1}{4\pi^2}\int_{\tilde{p}_{\mathrm{c}}\leq|p|\leq p_{\mathrm{c}}} \frac{\mathrm{d}p}{\mathrm{e}^{\beta(p^2-\mu_0)}-1} + o(1). \tag{2.16.15}$$

The remaining correction term can be estimated as

$$\frac{1}{4\pi^2}\int_{\tilde{p}_{\mathrm{c}}\leq|p|\leq p_{\mathrm{c}}} \frac{\mathrm{d}p}{\mathrm{e}^{\beta(p^2-\mu_0)}-1} \lesssim \frac{1}{\beta}\int_{\beta\tilde{p}_{\mathrm{c}}^2}^{\beta p_{\mathrm{c}}^2} \frac{\mathrm{d}q}{q-\beta\mu_0} = \frac{1}{\beta}\ln\left(\frac{\beta p_{\mathrm{c}}^2-\beta\mu_0}{\beta\tilde{p}_{\mathrm{c}}^2-\beta\mu_0}\right). \tag{2.16.16}$$

In combination, the above estimates show that

$$\frac{1}{|\Lambda|}F(\beta, N, |\Lambda|) \geq \mu_0\rho + \frac{1}{4\beta\pi^2}\int_{\mathbb{R}^2} \ln\left(1 - \mathrm{e}^{-\beta(p^2-\mu_0)}\right) \mathrm{d}p - \frac{1}{|\Lambda|}\sum_{i=1}^{5} Z^{(i)} - o(1)$$
$$+ \frac{4\pi}{|\ln a^2\rho|}\left(2\rho^2 - \rho_{\mathrm{s}}^2\right), \tag{2.16.17}$$

where

$$\begin{aligned} Z^{(5)} := &- \text{const.}\,(\kappa - \kappa')\frac{|\Lambda|}{\beta}\int_{\mathbb{R}^2} \ln\left(1 - \mathrm{e}^{-\beta(p^2-\mu_0)}\right) \mathrm{d}p \\ &- \frac{|\Lambda|}{\kappa'\beta^2}\int_{|p|^2 \geq \kappa'\beta/s^2} \ln\left(1 - \mathrm{e}^{-p^2}\right) \mathrm{d}p \\ &+ \frac{\text{const.}\,|\Lambda|\rho^2}{|\ln a^2\rho|}\left(\frac{1}{C} + \frac{1}{\beta\rho}\ln\left(\frac{\beta p_{\mathrm{c}}^2 - \beta\mu_0}{\beta\tilde{p}_{\mathrm{c}}^2 - \beta\mu_0}\right) + \frac{1}{(\beta\rho)^2}\ln^2\left(\frac{\beta p_{\mathrm{c}}^2 - \beta\mu_0}{\beta\tilde{p}_{\mathrm{c}}^2 - \beta\mu_0}\right)\right). \end{aligned} \tag{2.16.18}$$

Note that the right-hand side of (2.16.17) has the desired form: The sum of the first two terms on the right-hand side equals the free energy of non-interacting bosons $f_0(\beta, \rho)$ since μ_0 is given by (1.2.7). The last term in (2.16.17) is the desired interaction energy. It remains to choose the parameters in the error terms and show that they are of lower order than this interaction energy.

2.17 Minimizing the error terms

In this section we show how to choose the parameters in order to optimize the error terms of the lower bound.

To simplify the notation, we replace the factor $1/16$ in the definition of τ from (2.15.17) by one, i.e., we redefine

$$\tau = -\beta\mu_0 + \beta p_{\mathrm{c}}^2 \quad \text{and denote} \quad \tilde{\tau} = -\beta\mu_0 + \beta\tilde{p}_{\mathrm{c}}^2. \tag{2.17.1}$$

For brevity, let us introduce the notation

$$\sigma := |\ln a^2\rho|. \tag{2.17.2}$$

Similarly as in the three-dimensional case the following terms are relevant for the minimization: p_{c}^4 from $Z^{(1)}$, $\rho^2\sigma^{-1}(\kappa + R/s)$ and $\rho^2\sigma^{-1}(\beta\rho)^{1/2}(R^2\rho)^{-2}(\tau\sigma)^{-1/4}$ from $Z^{(4)}$ as well as

$$-\frac{1}{\kappa'\beta^2}\int_{|p|^2 \geq \kappa'\beta/s^2} \ln\left(1 - \mathrm{e}^{-p^2}\right) \mathrm{d}p \tag{2.17.3}$$

from $Z^{(5)}$. It turns out, however, that in the two-dimensional case the additional error terms $\rho^2\sigma^{-1}(R^2\rho)^{1/3}$ from $Z^{(4)}$ and $\rho^2\sigma^{-1}\ln(\tau/\tilde{\tau})/(\beta\rho)$ from $Z^{(5)}$ are also relevant for choosing the parameters. The constraints on the parameters, that is, $p_c \leq 1/s$, $s \gg R$, $s^2 \ll \kappa\beta$, $R_0^2/R^2 \ll \kappa$, $b \gg 1/p_c$, $b \gg R$ and $b \gg \beta^{1/2}$ will be automatically satisfied with the choice of the parameters below. The same is true for (2.13.28) and (2.13.35), which have to be obeyed by the parameter R. Since R appears in these expressions only in the argument of the logarithm, we still have quite some freedom in its choice.

In order for (2.17.3) to be small, we require that $s^2 \ll \kappa'\beta$, with κ' defined in (2.9.21). This is equivalent to $s^2 \ll \kappa\beta$, since we will choose $R_0^2/R^2 \ll \kappa$. If we take $\kappa' = (1+\delta)s^2\beta^{-1}\ln\sigma$ for some $\delta > 0$, (2.17.3) is bounded by $(s^2\beta)^{-1}\sigma{-}1-\delta$, which will be negligible compared to the other terms. We can now optimize the term $\rho^2\sigma^{-1}(\kappa + R/s)$ over s resulting in the choice

$$s = \left(\frac{\beta R}{\ln\sigma}\right)^{1/3}. \tag{2.17.4}$$

With this choice of s the error term becomes

$$\frac{\rho^2}{\sigma}\left((1+\delta)\frac{s^2\ln\sigma}{\beta} + \frac{R}{s}\right) \sim \frac{\rho^2}{\sigma}\left(\frac{R^2\ln\sigma}{\beta}\right)^{1/3}. \tag{2.17.5}$$

Among the main terms there are now only three terms left that depend on R, namely (2.17.5), $\rho^2\sigma^{-1}(R^2\rho)^{1/3}$ and $\rho^2\sigma^{-1}(\beta\rho)^{1/2}(R^2\rho)^{-2}(\tau\sigma)^{-1/4}$. Denoting

$$d = 1 + \left(\frac{\ln\sigma}{\beta\rho}\right)^{1/3} \sim 1 + \left(\frac{\beta_c}{\beta}\right)^{1/3}, \tag{2.17.6}$$

we write the sum of the first two terms as $\rho^2\sigma^{-1}(R^2\rho)^{1/3}d$. Hence, the optimal choice of R is

$$(R^2\rho)^{1/3} = \frac{(\beta\rho)^{1/14}}{d^{1/7}(\tau\sigma)^{1/28}} \tag{2.17.7}$$

and the resulting error term reads

$$\frac{\rho^2}{\sigma}(R^2\rho)^{1/3}d = \frac{\rho^2}{\sigma}d^{6/7}\left(\frac{(\beta\rho)^2}{\tau\sigma}\right)^{1/28}. \tag{2.17.8}$$

We are thus left with the following three error terms

$$\begin{aligned}
A_1 &= \frac{\rho^2}{\sigma}\frac{1}{\beta\rho}\ln\left(\frac{\tau}{\tilde{\tau}}\right) = \frac{\rho^2}{\sigma}\frac{1}{\beta\rho}\ln\left(\frac{\beta p_{\mathrm{c}}^2 - \ln(1-\mathrm{e}^{-4\pi\beta\rho})}{\beta\tilde{p}_{\mathrm{c}}^2 - \ln(1-\mathrm{e}^{-4\pi\beta\rho})}\right),\\
A_2 &= p_{\mathrm{c}}^4,\\
A_3 &= \frac{\rho^2}{\sigma}d^{6/7}\left(\frac{(\beta\rho)^2}{\tau\sigma}\right)^{1/28}\\
&= \frac{\rho^2}{\sigma}\left(1+\left(\frac{\beta_{\mathrm{c}}}{\beta}\right)^{1/3}\right)^{6/7}\left(\frac{(\beta\rho)^2}{(\beta p_c^2 - \ln(1-\mathrm{e}^{-4\pi\beta\rho}))\sigma}\right)^{1/28}.
\end{aligned} \tag{2.17.9}$$

They depend solely on p_{c}, $\beta\rho$ and σ, as $\tilde{p}_{\mathrm{c}}$ is given explicitly in (2.16.14). By minimizing over p_{c} we therefore obtain the final error rate $\min_{p_{\mathrm{c}}}\{A_1 + A_2 + A_3\}$, which depends only on $\beta\rho$ and σ. Optimization turns out to lead to the choice

$$\beta p_{\mathrm{c}}^2 = \begin{cases} 0 & \text{if } 1 \lesssim 4\pi\beta\rho \le \ln\left(\frac{\sigma}{(\ln\sigma)^{30}}\right),\\ \frac{(\beta\rho)^{30}}{\sigma\ln^{28}((\beta\rho)^{30}/(\sigma\tilde{\tau}))} & \text{if } \ln\left(\frac{\sigma}{(\ln\sigma)^{30}}\right) \le 4\pi\beta\rho \lesssim \sigma^{1/59},\\ \left(\frac{(\beta\rho)^2}{\sigma}\right)^{29/57} & \text{if } \sigma^{1/59} \lesssim \beta\rho \lesssim \sigma^{1/2}. \end{cases} \tag{2.17.10}$$

The upper limit $\beta\rho \lesssim \sigma^{1/2}$ is a natural restriction, since the interaction term is comparable to the non-interacting free energy if $\beta\rho \sim \sigma^{1/2}$ (compare with (1.2.11)), and hence the perturbative argument, on which the proof of the lower bound is based, cannot be expected to work anymore in this regime. For $\beta\rho$ of the order $\sigma^{1/2}$ or larger an additional argument using the result at $T = 0$ [52] as a crucial ingredient will be given in Section 2.18 to complete the proof of the lower bound.

The parameters φ and C in the remaining error terms (which we did not need to consider for the choice of p_{c}) may be chosen according to

$$\frac{1}{\sigma} \ll \varphi \ll \frac{\beta\rho}{\sigma}, \quad 1 \ll C \ll \sigma \tag{2.17.11}$$

if $\beta\rho$ is such that $p_{\mathrm{c}} \neq 0$. In case $\beta\rho$ is so small that $p_{\mathrm{c}} = 0$, we find that the upper restrictions to φ and C do not apply anymore and the choice only needs to satisfy the lower ones.

We now explain how to arrive at the choice (2.17.10) of p_{c}. We start by discussing what can be expected. For $\beta\rho$ far below $\beta_{\mathrm{c}}\rho$, in a sense to be made precise below, we have that the (absolute value of the) chemical potential $-\beta\mu_0$ is large enough compared to σ^{-1} to control the term A_3 and even allows for the choice $p_{\mathrm{c}} = 0$, which means that A_1 and A_2

both vanish. This changes when $\beta\rho$ comes close to $\beta_c\rho$, where we need that βp_c^2 is larger than σ^{-1}. Here, only A_1 and A_3 have to be considered for the optimization, while A_2 is subleading. For $\beta\rho$ far above $\beta_c\rho$, the optimal error rate changes as the term A_1 becomes irrelevant and we optimize using the terms A_2 and A_3.

Consider first the case $p_c = 0$, which means $\tilde{p}_c = 0$ by the assumption $p_c \geq \tilde{p}_c$, which also means $e^{4\pi\beta\rho} \leq \sigma$ or $\beta \leq \beta_c$. This implies $A_1 = A_2 = 0$ as well as $\tau = -\beta\mu_0 = -\ln(1 - e^{-4\pi\beta\rho})$. The remaining error term is given by

$$A_3 \lesssim \frac{\rho^2}{\sigma}\left(\frac{\beta_c}{\beta}\right)^{2/7}\left(\frac{(\beta\rho)^2}{\sigma\, e^{-4\pi\beta\rho}}\right)^{1/28}. \tag{2.17.12}$$

It can be read off that $e^{4\pi\beta\rho} \lesssim \sigma/(\ln\sigma)^2$ is the upper limit for this error to be smaller than the interaction scale, which is much smaller than the critical inverse temperature, $e\,4\pi\beta_c\rho = \sigma$. Hence, we need to choose a non-zero p_c already well above the critical temperature.

Next, we consider the case $p_c \neq 0$. This will be the case only in the regime $\beta \gtrsim \beta_c$, hence d in (2.17.6) satisfies $d \sim 1$. Since we have three main error terms to consider, there are three different possibilities of how to obtain the optimal p_c, out of which only two will be relevant. The first way of choosing p_c is obtained by optimizing A_1 and A_3. This leads to the equation

$$\frac{1}{\beta\rho}\ln\left(\frac{\tau}{\tilde{\tau}}\right) = \left(\frac{(\beta\rho)^2}{\sigma\tau}\right)^{1/28}, \tag{2.17.13}$$

which, to leading order, is solved by

$$\tau = \beta p_c^2 - \beta\mu_0 = \frac{(\beta\rho)^{30}}{\sigma\ln^{28}\left(\frac{(\beta\rho)^{30}}{\sigma\tilde{\tau}}\right)}. \tag{2.17.14}$$

As mentioned before, the reason for switching to $p_c \neq 0$ is that $-\beta\mu_0$ becomes too small in order to control the term A_3 (i.e., to ensure that A_3 is smaller than the interaction scale ρ^2/σ). Therefore, we can take the right-hand side of (2.17.14) as the defining equation for βp_c^2 and neglect the term $-\beta\mu_0$. The error terms with this choice of p_c become

$$\begin{aligned} A_1 \sim A_3 &\lesssim \frac{\rho^2}{\sigma}\frac{1}{\beta\rho}\ln\left(\frac{(\beta\rho)^{30}}{\sigma\tilde{\tau}\ln^{28}((\beta\rho)^{30}/(\sigma\tilde{\tau}))}\right), \\ A_2 &\lesssim \frac{\rho^2}{\sigma}\frac{(\beta\rho)^{58}}{\sigma\ln^{56}((\beta\rho)^{30}/(\sigma\tilde{\tau}))}. \end{aligned} \tag{2.17.15}$$

Note that $A_3 = A_1$ to leading order by our choice of p_c and that A_2 is indeed of lower order than A_1 or A_3 for $\beta\rho \sim \beta_c\rho$.

Now we can compare the term A_1 from (2.17.15) to the term A_3 we obtained by choosing $p_c = 0$ (from (2.17.12)) to determine the point at which we switch to $p_c \neq 0$ as given in (2.17.14). This gives

$$\left(\frac{(\beta\rho)^2}{\sigma\, e^{-4\pi\beta\rho}}\right)^{1/28} = \frac{1}{\beta\rho} \ln\left(\frac{(\beta\rho)^{30}}{\sigma\tilde{\tau} \ln^{28}((\beta\rho)^{30}/(\sigma\tilde{\tau}))}\right), \tag{2.17.16}$$

which we solve to leading order by

$$4\pi\beta\rho = \ln\left(\frac{\sigma}{(\ln\sigma)^{30}}\right). \tag{2.17.17}$$

For this value of $\beta\rho$ we switch to p_c as given in (2.17.14).

It is clear, however, that for larger $\beta\rho$ the term A_2 from (2.17.15) will become larger than A_1 or A_3 as it is increasing in $\beta\rho$. The point at which this happens is given by the solution of the equation

$$\frac{1}{\beta\rho} \ln\left(\frac{(\beta\rho)^{30}}{\ln^{28}(\beta\rho)^{30}}\right) = \frac{(\beta\rho)^{58}}{\sigma \ln^{56}(\beta\rho)^{30}}. \tag{2.17.18}$$

To leading order we solve it by $\beta\rho = \sigma^{1/59}$. From here on, we use the second way of optimizing p_c by considering the terms A_2 and A_3 with the result

$$\beta p_c^2 = \left(\frac{(\beta\rho)^2}{\sigma}\right)^{29/57}. \tag{2.17.19}$$

The error terms then become

$$\begin{aligned} A_1 &\lesssim \frac{\rho^2}{\sigma}\frac{1}{\beta\rho} \ln\left((\beta\rho)^{58/57}\sigma^{28/57}\right), \\ A_2 &\lesssim \frac{\rho^2}{\sigma}\left(\frac{(\beta\rho)^2}{\sigma}\right)^{1/57}. \end{aligned} \tag{2.17.20}$$

Note that from this form of A_2 we can also read off the natural upper limit $\beta\rho \ll \sigma^{1/2}$ for the error terms to be small.

2.18 Uniformity in the temperature

For $\beta\rho$ of the order $\sigma^{1/2}$ or larger we apply a technique that uses in an essential way the result for the ground state energy [52]. This will allow us to obtain the desired uniformity in $\beta\rho$, as already mentioned in the previous section.

Starting from the original Hamiltonian with potential v (which we denoted by H_N), we use Lemma 4 to obtain

$$H_N \geq \sum_{j=1}^{N} \Big[-\nabla_j (1-(1-\kappa))\chi(p_j)^2)\nabla_j + (1-\epsilon)(1-\kappa) U_R(d(x_j, x_{\mathrm{NN}}^{J_j}(x_j))) \\ - \frac{1}{\epsilon} \int_{\mathbb{R}_+} U_R(t) t \,\mathrm{d}t \sum_{i \in J_j} w_R(x_j - x_i) \Big]. \tag{2.18.1}$$

Strictly speaking we should work with a symmetrization of the right-hand side of (2.18.1) since the potential that we obtained from Lemma 4 is not permutation symmetric. As already mentioned before, this does not need to concern us since we only consider expectation values in bosonic states. The last term in (2.18.1) can be estimated using the integral condition on U_R (from (2.8.3)), the decay property of g (which was introduced in (2.12.9)) as well as the definition of J_j:

$$\sum_{j=1}^{N} \frac{1}{\epsilon} \int_{\mathbb{R}_+} U_R(t) t \,\mathrm{d}t \sum_{i \in J_j} w_R(x_j - x_i) \\ \leq \frac{1}{\epsilon \ln(R/a)} \sum_{j=1}^{N} \sum_{i \in J_j} \frac{R^2}{s^4} g(d(x_i, x_j)/s) \lesssim \frac{N}{\epsilon \ln(R/a) s^2}. \tag{2.18.2}$$

More precisely, in order to obtain the second inequality we partition space into annuli Ω_k, $k = 0, 1, 2, \ldots$, centered at x_j of radius $(k+1)s$ and thickness s. Then we estimate the particle number in each annulus by using $d(x_i, x_k) \geq R/5$ for $i, k \in J_j$ and an easy counting argument. For Ω_0 (which is just the disc of radius s), we find as an upper bound for the particle number

$$\frac{(s + R/10)^2}{(R/5)^2} \lesssim \left(\frac{s}{R}\right)^2. \tag{2.18.3}$$

Here, we also used $R/5 \leq s$. For $k \neq 0$, the corresponding expression is

$$\frac{((k+1)s + R/10)^2 - (ks - R/10)^2}{(R/5)^2} = 5\frac{(1+2k)s(R+5s)}{R^2} \leq 50 \frac{(1+2k)s^2}{R^2} \\ \lesssim k \left(\frac{s}{R}\right)^2. \tag{2.18.4}$$

The decay property of g says that for fixed $\alpha > 0$ and for $x \in \Omega_k$ we have $g(d(x, x_j)/s) \lesssim k^{-\alpha}$.

Hence, we obtain

$$\begin{aligned}\sum_{i\in J_j} g(d(x_i,x_j)/s) &= \sum_{k=0}^{\infty} \sum_{i\in J_j, x_i\in\Omega_k} g(d(x_i,x_j)/s)\\ &\leq \sum_{k=0}^{\infty} \#\{i\in J_j : x_i\in\Omega_k\} \sup_{x\in\Omega_k} g(d(x,x_j)/s)\\ &\lesssim \sum_{k=0}^{\infty} k\left(\frac{s}{R}\right)^2 \frac{1}{k^\alpha} \lesssim \left(\frac{s}{R}\right)^2. \end{aligned} \tag{2.18.5}$$

To find a lower bound for the remaining terms we use the main result from [52] (for the choice $\kappa = \sigma^{-1/5}, R\rho^{1/2} = \sigma^{-1/10}$) and find

$$\sum_{j=1}^{N}\left(-\frac{\kappa}{2}\Delta_j + (1-\epsilon)(1-\kappa)U_R(d(x_j, x_{\mathrm{NN}}^{J_j}(x_j)))\right) \geq \frac{4\pi N\rho}{\sigma}\left(1-\epsilon-\frac{\mathrm{const}}{\sigma^{1/5}}\right). \tag{2.18.6}$$

Even though the result in [52] was for Neumann boundary conditions and the full nearest-neighbor interaction, it is straight-forward to check that it also holds in our case. The ground state of the non-interacting system for periodic boundary conditions is also a constant, and the difference between the nearest-neighbor interaction in that paper and our interaction can be bounded by a constant times $N^2(R^2/L^2)^2\|U_R\|_\infty$. A term like this is already contained in the original estimate in [52, Eqs. (3.18) and (3.19)]. In [52] the potential $U_R(d(x_j, x_{\mathrm{NN}}(x_j)))$ is used, where the nearest neighbor was determined among all other particles while here we only look for the nearest neighbor in the set J_j. The related error can be controlled with an estimate for the probability of finding a particle coordinate that is not contained in the set J_j. It is straight-forward to check that this probability is bounded by a constant times $N^2(R^2/L^2)^2$ times the L^∞ norm of the potential U_R.

The above considerations allow us to show that

$$H_N \geq \sum_{j=1}^{N} \ell\left(\sqrt{-\Delta_j}\right) + \frac{4\pi N\rho}{\sigma}\left(1-\epsilon-\frac{\mathrm{const.}}{\sigma^{1/5}} - \frac{\mathrm{const.}}{\epsilon s^2\rho}\right), \tag{2.18.7}$$

where $\ell(p) = p^2(1-\sigma^{-1/5}/2-(1-\sigma^{-1/5})\chi(p)^2)$. We already inserted the choice $\kappa = \sigma^{-1/5}$ from above. Next, we consider the free energy related to H_N, introduce the chemical potential μ_0 and drop the restriction on the particle number. When we also take the thermodynamic limit we find

$$f(\beta,\rho) \geq f_0(\beta,\rho) + \text{const.}\frac{1}{\beta\sigma^{1/5}}\int_{\mathbb{R}^2} \ln\left(1-\mathrm{e}^{-\beta(p^2-\mu_0)}\right)\,\mathrm{d}p \\ + \frac{1}{\beta^2\sigma^{1/5}}\int_{p^2\geq\beta/(s^2\sigma^{1/5})} \ln\left(1-\mathrm{e}^{-p^2/2}\right)\,\mathrm{d}p + \frac{4\pi\rho^2}{\sigma}\left(1-\epsilon-\frac{\text{const.}}{\sigma^{1/5}}-\frac{\text{const.}}{\epsilon s^2\rho}\right). \tag{2.18.8}$$

As before, we require $s^2\sigma^{1/5}/\beta \ll 1$ for the correction term to the non-interacting free energy to be small. If we choose

$$\frac{s^2}{\beta} = \frac{1}{2\delta\sigma^{1/5}\ln\sigma} \tag{2.18.9}$$

for some $\delta > 0$ this error term is bounded from above by a constant times $\beta^{-2}\sigma^{-1/5-\delta}$ and will be negligible compared to other terms. Optimization over ϵ yields

$$\epsilon = \sqrt{\frac{1}{s^2\rho}}. \tag{2.18.10}$$

Therefore, we have

$$f(\beta,\rho) \geq f_0(\beta,\rho) + \frac{4\pi\rho^2}{\sigma}\left(1-\text{const.}\left[\frac{\sigma^{4/5}}{(\beta\rho)^2}+\frac{1}{\sigma^{1/5}}+\frac{\sigma^{1/10}(\ln\sigma)^{1/2}}{(\beta\rho)^{1/2}}\right]\right). \tag{2.18.11}$$

It remains to estimate the term depending on the critical temperature as

$$\frac{4\pi\rho^2}{\sigma}\left(1-\left[1-\frac{\beta_c}{\beta}\right]_+^2\right) \lesssim \frac{\rho^2}{\sigma}\frac{\beta_c}{\beta}. \tag{2.18.12}$$

Hence, the total error to consider is bounded from above by a constant times

$$\frac{\rho^2}{\sigma}\left(\frac{\sigma^{4/5}}{(\beta\rho)^2}+\frac{1}{\sigma^{1/5}}+\frac{\ln\sigma}{\beta\rho}+\frac{\sigma^{1/10}(\ln\sigma)^{1/2}}{(\beta\rho)^{1/2}}\right). \tag{2.18.13}$$

The optimal point at which we switch from the error given in (2.17.20) to this error is determined by comparing the term A_2 with the first term in (2.18.13). This leads to the equation

$$\frac{\sigma^{4/5}}{(\beta\rho)^2} = \left(\frac{(\beta\rho)^2}{\sigma}\right)^{1/57}, \tag{2.18.14}$$

which is solved by $\beta\rho = \sigma^{233/580}$. If $\beta\rho$ is larger than or equal to this value we use the result derived in this section.

In conclusion, by combining the results from the previous estimates in (2.17.12), (2.17.15), (2.17.20) and (2.18.13), we have shown that the bound

$$f(\beta,\rho) \geq f_0(\beta,\rho) + \frac{4\pi\rho^2}{\sigma}\left(2 - \left[1 - \frac{\beta_c}{\beta}\right]_+^2\right)(1 - o(1)) \tag{2.18.15}$$

holds uniformly in $\beta\rho \gtrsim 1$, where

$$o(1) \lesssim \begin{cases} \left(\frac{\ln\sigma}{\beta\rho}\right)^{2/7}\left(\frac{(\beta\rho)^2}{-\sigma\ln(1-e^{-4\pi\beta\rho})}\right)^{1/28} & \text{if } 1 \lesssim 4\pi\beta\rho \leq \ln(\sigma/(\ln\sigma)^{30}), \\ \frac{1}{\beta\rho}\ln\left(\frac{(\beta\rho)^{30}}{\sigma\tilde{\tau}\ln^{28}((\beta\rho)^{30}/(\sigma\tilde{\tau}))}\right) + \frac{(\beta\rho)^{58}}{\sigma\ln^{56}((\beta\rho)^{30}/(\sigma\tilde{\tau}))} & \text{if } \ln(\sigma/(\ln\sigma)^{30}) \leq 4\pi\beta\rho \lesssim \sigma^{1/59}, \\ \frac{1}{\beta\rho}\ln\left((\beta\rho)^{58/57}\sigma^{28/57}\right) + \left(\frac{(\beta\rho)^2}{\sigma}\right)^{1/57} & \text{if } \sigma^{1/59} \lesssim \beta\rho \lesssim \sigma^{233/580}, \\ \frac{\sigma^{4/5}}{(\beta\rho^2)} + \frac{1}{\sigma^{1/5}} + \frac{\sigma^{1/10}(\ln\sigma)^{1/2}}{(\beta\rho)^{1/2}} & \text{if } \sigma^{233/580} \lesssim \beta\rho. \end{cases} \tag{2.18.16}$$

The largest error occurs in the second regime if $\beta\rho \sim \beta_c\rho$, and is given by

$$\frac{1}{\ln\sigma}\ln\left(\frac{(\ln\sigma)^{30}}{\ln^{28}((\ln\sigma)^{30})}\right) + \frac{(\ln\sigma)^{58}}{\sigma\ln^{56}((\ln\sigma)^{30})} \lesssim \frac{\ln\ln\sigma}{\ln\sigma} \tag{2.18.17}$$

for σ large. We note that $\tilde{\tau} \sim \sigma^{-1}$ in this case, which follows from (1.2.7), (2.16.14) and (2.17.1). This concludes the proof of Theorem 2.

2.A Proof of Dyson Lemma in two dimensions

The proof of Lemma 4 can be obtained by combining the ideas of the proofs of [45, Lemma 7] and [70, Lemma 2]. Since the proof of the two-dimensional version of the relevant Lemma in [45] is not spelled out explicitly, we give the proof of Lemma 4 here. For simplicity of the notation, we shall drop the ~ for v and a.

Proof of Lemma 4. Given the points y_i, we partition the torus Λ into Voronoi cells

$$\mathcal{B}_i = \{x \in \Lambda : d(x,y_i) \leq d(x,y_k) \text{ for all } k \neq i\}. \tag{2.A.1}$$

For any $\psi \in H^1(\Lambda)$ denote by ξ the function with Fourier transform $\hat{\xi}(p) = \chi(p)\hat{\psi}(p)$. To obtain (2.8.4) it is enough to show that

$$\begin{aligned}\int_{\mathcal{B}_i} |\nabla\xi(x)|^2 + \frac{1}{2}v(d(x,y_i))|\psi(x)|^2\,\mathrm{d}x \geq (1-\epsilon)\int_{\mathcal{B}_i} U_R(d(x,y_i))|\psi(x)|^2\,\mathrm{d}x \\ - \frac{1}{\epsilon}\int_{\mathbb{R}_+} U_R(t)t\,\mathrm{d}t\int_\Lambda w_R(x-y_i)|\psi(x)|^2\,\mathrm{d}x.\end{aligned} \tag{2.A.2}$$

Using the positivity of v and summing over i, as well as realizing that for $x \in \mathcal{B}_i$ we have $y_i = y_{\mathrm{NN}}(x)$, we obtain (2.8.4):

$$\begin{aligned}\int_\Lambda |\nabla\xi(x)|^2 + \frac{1}{2}\sum_i v(d(x,y_i))|\psi(x)|^2\,\mathrm{d}x &= \sum_i \int_{\mathcal{B}_i}\left(|\nabla\xi(x)|^2 + \frac{1}{2}v(d(x,y_i))|\psi(x)|^2\right)\mathrm{d}x \\ &\geq \sum_i (1-\epsilon)\int_{\mathcal{B}_i} U_R(d(x,y_i))|\psi(x)|^2\,\mathrm{d}x - \frac{1}{\epsilon}\int_{\mathbb{R}_+} U_R(t)t\,\mathrm{d}t \sum_i \int_\Lambda w_R(x-y_i)|\psi(x)|^2\,\mathrm{d}x \\ &= (1-\epsilon)\int_\Lambda U_R(d(x,y_{\mathrm{NN}}(x)))|\psi(x)|^2\,\mathrm{d}x - \frac{1}{\epsilon}\int_{\mathbb{R}_+} U_R(t)t\,\mathrm{d}t \int_\Lambda \sum_i w_R(x-y_i)|\psi(x)|^2\,\mathrm{d}x.\end{aligned} \tag{2.A.3}$$

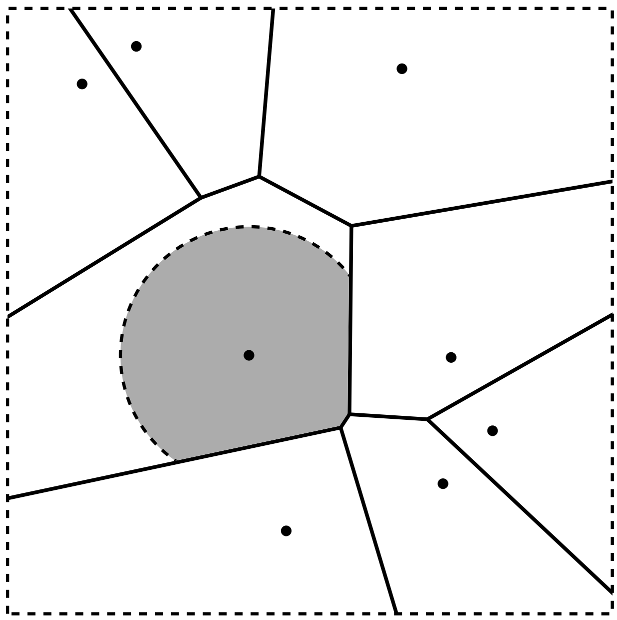

Figure 2.A.1: An example of a partition of a subset of Λ into Voronoi cells given by the y_i for $n = 8$. For one of the y_i the region $\mathcal{B}_R$ is shaded. Note that this image does not show the whole of Λ but merely a cutout (that does not respect the periodic boundary conditions).

We shall show that (2.A.2) actually holds with $\mathcal{B}_i$ replaced by the smaller set $\mathcal{B}_R = \mathcal{B}_i \cap \{x \in \Lambda : d(x,y_i) \leq R\}$ on the left-hand side of the inequality. Since the support of U_R is contained in the interval $[R_0, R]$, the integral over $\mathcal{B}_i$ on the right-hand side is also over $\mathcal{B}_R$. See Figure 2.A.1 for an illustration of the case $n = 8$. Take ζ to be a complex-valued function on the circle with L^2-norm one and by abuse of notation we shall use the same letter for the funtion on $\mathbb{R}^2$ taking values $\zeta(x/|x|)$. Recall the notation ϕ_v for the solution to the zero-energy scattering equation $(-\Delta + \frac{v}{2})\phi_v = 0$ on $\{|x| \leq R\}$ with boundary condition $\phi_v|_{|x|=R} = 1$.

Consider now the expression

$$A = \int_{\mathcal{B}_R} \zeta(x - y_i)\left(\nabla\bar{\xi}(x) \cdot \nabla\phi_v(x - y_i) + \frac{1}{2}v(d(x, y_i))\bar{\psi}(x)\phi_v(x - y_i)\zeta(x - y_i)\right) \mathrm{d}x. \quad (2.A.4)$$

An application of the Cauchy-Schwarz inequality gives

$$\begin{aligned} |A|^2 \leq &\int_{\mathcal{B}_R} \left(|\nabla\xi(x)|^2 + \frac{1}{2}v(d(x, y_i))|\psi(x)|^2\right) \mathrm{d}x \\ &\times \int_{\mathcal{B}_R} \left(|\nabla\phi_v(x - y_i)|^2 + \frac{1}{2}v(d(x, y_i))|\phi_v(x - y_i)|^2\right) |\zeta(x - y_i)|^2 \,\mathrm{d}x. \end{aligned} \quad (2.A.5)$$

In the second integral, we can replace the region $\mathcal{B}_R$ by the bigger one $\{d(x, y_i) \leq R\}$ for an upper bound. Since ϕ_v is radial, the angular integration over ζ contributes a factor of one. Using the definition of the scattering length, the remaining radial integration gives a factor $1/\ln(R/a)$. Thus,

$$|A|^2 \ln(R/a) \leq \int_{\mathcal{B}_R} \left(|\nabla\xi(x)|^2 + \frac{1}{2}v(d(x, y_i))|\psi(x)|^2\right) \mathrm{d}x, \quad (2.A.6)$$

which holds for any ζ with $\int_{\mathbb{S}^1} |\zeta|^2 = 1$.

For a lower bound, we note first that by integrating by parts we obtain

$$\begin{aligned} \int_{\mathcal{B}_R} \zeta(x - y_i)\nabla\bar{\xi}(x) \cdot \nabla\phi_v(x - y_i) \,\mathrm{d}x = &- \int_{\mathcal{B}_R} \bar{\xi}(x)\zeta(x - y_i)\Delta\phi_v(x - y_i) \,\mathrm{d}x \\ &+ \int_{\partial\mathcal{B}_R} \bar{\xi}(x)\zeta(x - y_i)n \cdot \nabla\phi_v(x - y_i) \,\mathrm{d}\omega_R, \end{aligned} \quad (2.A.7)$$

where we used the fact $\nabla\zeta(x) \cdot \nabla\phi_v(x) = 0$ (since ζ is defined on the circle and ϕ_v is radial), $\mathrm{d}\omega_R$ is the surface measure of the boundary of $\mathcal{B}_R$ and n is the outward unit normal. Note that $\xi(x) = \psi(x) - (2\pi)^{-1}h * \psi(x)$, where $h * \psi(x) = \int_\Lambda h(x - y)\psi(y) \,\mathrm{d}y$, as an easy calculation using the definition of h shows. If we insert this as well as (2.A.7) into the definition of A

and use the zero-energy scattering equation for ϕ_v, we obtain

$$\begin{aligned} A &= \int_{\partial\mathcal{B}_R} \left[\bar{\psi}(x) - (2\pi)^{-1}\overline{(h*\psi)}(x)\right] \zeta(x-y_i) n\cdot\nabla\phi_v(x-y_i)\,\mathrm{d}\omega_R \\ &\quad + \frac{1}{2\pi}\int_{\mathcal{B}_R} \overline{(h*\psi)}(x)\zeta(x-y_i)\Delta\phi_v(x-y_i)\,\mathrm{d}x \\ &= \int_{\partial\mathcal{B}_R} \bar{\psi}(x)\zeta(x-y_i)n\cdot\nabla\phi_v(x-y_i)\,\mathrm{d}\omega_R + \frac{1}{2\pi}\int_\Lambda \bar{\psi}(x)\int_{\mathcal{B}_R} h(y-x)\,\mathrm{d}\mu(y)\,\mathrm{d}x, \end{aligned} \tag{2.A.8}$$

where

$$\mathrm{d}\mu(x) = \zeta(x-y_i)\Delta\phi_v(x-y_i)\,\mathrm{d}x - n\cdot\nabla\phi_v(x-y_i)\zeta(x-y_i)\,\mathrm{d}\omega_R \tag{2.A.9}$$

is a measure supported in $\mathcal{B}_R$. It satisfies

$$\int_{\mathcal{B}_R}\mathrm{d}\mu(x) = \int_{\mathcal{B}_R}\zeta(x-y_i)\Delta\phi_v(x-y_i)\,\mathrm{d}x - \int_{\partial\mathcal{B}_R} n\cdot\nabla\phi_v(x-y_i)\zeta(x-y_i)\,\mathrm{d}\omega_R = 0, \tag{2.A.10}$$

as can be seen using again integration by parts. Moreover,

$$\int_{\mathcal{B}_R}\mathrm{d}|\mu| = 2\int_{\mathcal{B}_R}\Delta\phi_v(x-y_i)\,\mathrm{d}x \le 2\left(\int_{S^1}|\zeta|\right)\int_0^R \Delta\phi_v(r)r\,\mathrm{d}r \le \frac{2\sqrt{2\pi}}{\ln(R/a)}, \tag{2.A.11}$$

where we used the Cauchy-Schwarz inequality in the last step. Therefore, by invoking the definition of f_R from (2.8.2), we obtain

$$\left|\int_{\mathcal{B}_R} h(y-x)\,\mathrm{d}\mu(y)\right| = \left|\int_{\mathcal{B}_R}(h(y-x)-h(x-y_i))\,\mathrm{d}\mu(y)\right| \le \frac{2\sqrt{2\pi}}{\ln(R/a)} f_R(x-y_i). \tag{2.A.12}$$

This enables us to estimate the second term in (2.A.8) from below as

$$\begin{aligned} -\frac{1}{2\pi}\left|\int_\Lambda \bar{\psi}(x)\int_{\mathcal{B}_R} h(y-x)\,\mathrm{d}\mu(y)\,\mathrm{d}x\right| &\ge -\frac{1}{2\pi}\frac{2\sqrt{2\pi}}{\ln(R/a)}\int_\Lambda |\psi(x)| f_R(x-y_i)\,\mathrm{d}x \\ &\ge -\frac{1}{\ln(R/a)}\left(\int_\Lambda |\psi(x)|^2 w_R(x-y_i)\,\mathrm{d}x\right)^{1/2}, \end{aligned} \tag{2.A.13}$$

where we used again the Cauchy-Schwarz inequality as well as the definition of w_R from (2.8.2). Note that this bound is also independent of ζ, provided its L^2-norm equals one.

It remains to estimate the first term in (2.A.8). We define the set $\partial\tilde{\mathcal{B}}_R$ to be the part of $\partial\mathcal{B}_R$ that is at a distance R from y_i and assume that it is non-empty. In Figure 2.A.1 this set would correspond to the dashed arc. After the previous estimates, the second term in (2.A.8) is the only place where ζ is still present. For $\omega \in \mathbb{S}^1$, we choose

$$\zeta(\omega) = \begin{cases} \sqrt{R}\left(\int_{\partial\tilde{\mathcal{B}}_R} |\psi(x)|^2 \,\mathrm{d}\omega_R\right)^{-1/2} \psi(R\omega) & \text{if } R\omega \in \partial\tilde{\mathcal{B}}_R, \\ 0 & \text{otherwise,} \end{cases} \tag{2.A.14}$$

which satisfies $\int_{\mathbb{S}^1} |\zeta(\omega)|^2 \,\mathrm{d}\omega = 1$. In other words, we choose ζ to attain the value of ψ at those boundary points which are at a distance of R and zero elsewhere, while maintaining the proper normalization. Inserting this choice of ζ as well as the asymptotic solution for ϕ_v, we have

$$\int_{\partial\mathcal{B}_R} \bar{\psi}(x)\zeta(x-y_i) n \cdot \nabla\phi_v(x-y_i)\,\mathrm{d}\omega_R = \frac{1}{\sqrt{R}\ln(R/a)}\left(\int_{\partial\tilde{\mathcal{B}}_R} |\psi(x)|^2 \,\mathrm{d}\omega_R\right)^{1/2}. \tag{2.A.15}$$

Therefore,

$$|A| \geq \frac{1}{\ln(R/a)}\left[\frac{1}{\sqrt{R}}\left(\int_{\partial\tilde{\mathcal{B}}_R} |\psi(x)|^2 \,\mathrm{d}\omega_R\right)^{1/2} - \left(\int_\Lambda |\psi(x)|^2 w_R(x-y_i)\,\mathrm{d}x\right)^{1/2}\right]. \tag{2.A.16}$$

Another application of the Cauchy-Schwarz inequality gives for any $\epsilon > 0$

$$|A|^2 \ln(R/a) \geq \frac{1}{\ln(R/a)}\left[\frac{1-\epsilon}{R}\int_{\partial\tilde{\mathcal{B}}_R} |\psi(x)|^2 \,\mathrm{d}\omega_R - \frac{1}{\epsilon}\int_\Lambda |\psi(x)|^2 w_R(x-y_i)\,\mathrm{d}x\right]. \tag{2.A.17}$$

Hence, combining (2.A.6) and (2.A.17), we obtain

$$\begin{aligned} &\int_{\mathcal{B}_R} |\nabla\xi(x)|^2 + \frac{1}{2}v(d(x,y_i))|\psi(x)|^2 \,\mathrm{d}x \\ &\quad \geq \frac{1}{\ln(R/a)}\left[\frac{1-\epsilon}{R}\int_{\partial\tilde{\mathcal{B}}_R} |\psi(x)|^2 \,\mathrm{d}\omega_R - \frac{1}{\epsilon}\int_\Lambda |\psi(x)|^2 w_R(x-y_i)\,\mathrm{d}x\right]. \end{aligned} \tag{2.A.18}$$

In case $\partial\tilde{\mathcal{B}}_R$ is empty, the above inequality holds also true. Therefore we can relax the assumption on $\partial\tilde{\mathcal{B}}_R$. This proves the lemma for the special case of U_R being a radial δ function supported on the circle of radius R, i.e., $U_R(r) = (R\ln(R/a))^{-1}\delta(r-R)$. By replacing in the above inequality R by r, multiplying by $U_R(r)r\ln(r/a)$ and then finally integrating in r from R_0 to R, we obtain

$$\begin{aligned}
&\int_{\mathcal{B}_R} |\nabla\xi(x)|^2 + \frac{1}{2}v(d(x,y_i))|\psi(x)|^2 \, \mathrm{d}x \qquad (2.A.19)\\
&\geq \int_{R_0}^{R} U_R(r) r \ln(r/a) \left[\int_{\mathcal{B}_r} |\nabla\xi(x)|^2 + \frac{1}{2}v(d(x,y_i))|\psi(x)|^2 \, \mathrm{d}x \right] \mathrm{d}r \\
&\geq \int_{R_0}^{R} U_R(r) r \left[\frac{1-\epsilon}{r} \int_{\partial\tilde{\mathcal{B}}_r} |\psi(x)|^2 \, \mathrm{d}\omega_r - \frac{1}{\epsilon} \int_{\Lambda} |\psi(x)|^2 w_r(x-y_i) \, \mathrm{d}x \right] \mathrm{d}r \\
&\geq (1-\epsilon) \int_{R_0}^{R} U_R(r) \int_{\partial\tilde{\mathcal{B}}_r} |\psi(x)|^2 \, \mathrm{d}\omega_r \, \mathrm{d}r - \frac{1}{\epsilon} \int_{\mathbb{R}_+} U_R(t) t \, \mathrm{d}t \int_{\Lambda} |\psi(x)|^2 w_R(x-y_i) \, \mathrm{d}x \\
&= (1-\epsilon) \int_{\mathcal{B}_R} U_R(d(x,y_i)) |\psi(x)|^2 \, \mathrm{d}x - \frac{1}{\epsilon} \int_{\mathbb{R}_+} U_R(t) t \, \mathrm{d}t \int_{\Lambda} |\psi(x)|^2 w_R(x-y_i) \, \mathrm{d}x,
\end{aligned}$$

where we used (2.8.3) in the first inequality and the fact that w_r is monotone increasing in r in the last inequality. □

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3 Upper bound on the free energy

Simon Mayer and Robert Seiringer

We prove an upper bound on the free energy of an interacting two-dimensional homogeneous Bose gas in a dilute setting. We show that for $a^2\rho \ll 1$ and $\beta\rho$ of order one or larger the free energy differs from the free energy of the non-interacting system by a correction term $4\pi\rho^2|\ln a^2\rho|^{-1}(2-[1-\beta_c/\beta]_+^2)$, where a is the scattering length of the two-body interaction potential, ρ is the density, β is the inverse temperature and β_c is the inverse critical Berezinskii–Kosterlitz–Thouless temperature for superfluidity. Together with the corresponding matching lower bound proved in Chapter 2 this shows equality in the asymptotic expansion.

3.1 Statement of the upper bound

Theorem 3 (Upper bound on the free energy)**.** *Assume that the interaction potential satisfies* $v \geq 0$ *and has a finite scattering length. As* $a^2\rho \to 0$ *with* $\beta\rho \gtrsim 1$*, we have*

$$f(\beta,\rho) \leq f_0(\beta,\rho) + \frac{4\pi\rho^2}{|\ln a^2\rho|}\left(2 - \left[1 - \frac{\beta_c(\rho,a)}{\beta}\right]_+^2\right)(1 + o(1)), \tag{3.1.1}$$

where

$$o(1) \lesssim \frac{\ln\ln|\ln a^2\rho|}{\ln|\ln a^2\rho|}. \tag{3.1.2}$$

Here, $[\,\cdot\,]_+ = \max\{\,\cdot\,,0\}$ *denotes the positive part and the inverse critical temperature* $\beta_c(\rho,a)$ *is defined in* (1.1.7)*.*

3.2 Sketch of the proof

The basis of the proof of Theorem 3 is the variational principle for the free energy, which is presented in Section 3.3 below. An upper bound is obtained by inserting a suitable admissible trial state into the free energy functional that gives us the leading order contribution $f_0(\beta,\rho-\rho_0) + 4\pi|\ln a^2\rho|^{-1}(2\rho^2 - \rho_0^2)$ for any $0 \leq \rho_0 \leq \rho$. As mentioned in Remark 5 in Section 1.2 and explained in more detail in Section 1.5, the optimal choice for ρ_0 turns out to be

$$\rho_s = \rho\left[1 - \frac{\beta_c}{\beta}\right]_+, \tag{3.2.1}$$

which in turn leads to the form of the upper bound as given in Theorem 3.

The trial state that we are going to insert into the free energy functional is built up out of three parts. The first part is the thermal Gibbs state of the non-interacting system at density $\rho - \rho_0$, the second part is a coherent state of the $p = 0$ mode with density ρ_0 and the third part is a product function, where each factor is given by the solution to the zero-energy scattering equation evaluated at the distance between all pairs of particles (so called Jastrow factor [34]). We remark that compared to the proof of the lower bound in Chapter 2, it is not necessary here to use a c-number substitution for more than one mode to obtain the correct contribution for the interaction term. We then partition the square $[0,L]^2$ into $(L/\ell)^2$ smaller boxes of size ℓ and construct a state on the box of size L that is a tensor product of identical copies of the above trial state (up to translation) on the small boxes of size ℓ. This enables us to effectively decouple the thermodynamic limit and the dilute limit.

We remark that this strategy of proving the upper bound of the dilute asymptotics in the two-dimensional setting is simpler than the proof of [79, Theorem 1] in three dimensions. In our case it turns out that the parameters that appear in correction terms coming from estimating the norm of the trial state can be chosen in a way such that they are smaller than the scale of the interaction energy, $\rho^2|\ln a^2\rho|^{-1}$. This was much harder to achieve in the three-dimensional case.

3.3 Preliminary tools

In this subsection we present a few tools that will be essential to the method of proof. First we present a lemma for approximating sums by integrals, then a lemma about properties of the scattering solution and finally we discuss the variational definition of the free energy in the canonical and grand canonical setting, as well as a lemma that proves equality of these two definitions in the thermodynamic limit.

Lemma 9 (Two-dimensional version for periodic boundary conditions of Lemma 4 in [69])**.** *Let $f : \mathbb{R}_+ \to \mathbb{R}_+$ be a monotone decreasing function and $-\Delta$ the Laplacian with periodic boundary conditions on the square of side length ℓ. Then we have*

$$\frac{\ell^2}{4\pi^2}\int_{\mathbb{R}^2}\left(1-\frac{4}{\ell|p|}\right)f(p^2)\,\mathrm{d}p \le \operatorname{Tr} f(-\Delta) \le \frac{\ell^2}{4\pi^2}\int_{\mathbb{R}^2}\left(1+\frac{4}{\ell|p|}\right)f(p^2)\,\mathrm{d}p + f(0). \quad (3.3.1)$$

Proof. Note that

$$\operatorname{Tr} f(-\Delta) = \sum_{p\in(2\pi/\ell)\mathbb{Z}^2} f(p^2) \quad (3.3.2)$$

since the spectrum of the Laplacian with periodic boundary conditions is $\sigma(-\Delta) = [(2\pi/\ell)\mathbb{Z}]^2$. Consider a decomposition of the plane into squares of side length $2\pi/\ell$. Since f is monotone decreasing, we have that the smallest value of $f(p^2)$ for p in such a square is obtained at the corner that is farthest away from the origin. Thus we see that the sum over the points p that do not lie on a coordinate axis (i.e., the points $p = (p_1, p_2)$ for which neither $p_1 \neq 0$ nor $p_2 \neq 0$) is the lower Riemann sum to the integral of f over the plane:

$$\sum_{p\in(2\pi/\ell)\mathbb{Z}^2} f(p^2) \le \frac{\ell^2}{4\pi^2}\int_{\mathbb{R}^2} f(p^2)\,\mathrm{d}p + \sum_{p\in\text{axes}} f(p^2). \quad (3.3.3)$$

Similarly, we can estimate the sum over the axes by a one-dimensional integral as

$$\sum_{p\in\text{axes}} f(p^2) = f(0) + 4\sum_{p\in(2\pi/\ell)\mathbb{N}} f(p^2) \le f(0) + \frac{2\ell}{\pi}\int_0^\infty f(p^2)\,\mathrm{d}p = f(0) + \frac{\ell}{\pi^2}\int_{\mathbb{R}^2}\frac{f(p^2)}{|p|}\,\mathrm{d}p. \quad (3.3.4)$$

In conclusion, we have

$$\sum_{p\in(2\pi/\ell)\mathbb{Z}^2} f(p^2) \leq \frac{\ell^2}{4\pi^2}\int_{\mathbb{R}^2}\left(1+\frac{4}{\ell|p|}\right) f(p^2)\,\mathrm{d}p + f(0). \tag{3.3.5}$$

For the lower bound, we proceed in a similar fashion. We use that $f(p^2)$ attains its largest value at the corners that lie closest to the origin and have that the sum over all points is the upper Riemann sum to the integral over the plane without the region

$$\mathcal{G} = \left\{(p_1,p_2)\in\mathbb{R}^2 : 0 < p_1 < \frac{2\pi}{\ell} \text{ or } -\frac{2\pi}{\ell} < p_2 < 0\right\} \tag{3.3.6}$$

which means

$$\int_{\mathbb{R}^2} f(p^2)\,\mathrm{d}p = \int_{\mathbb{R}^2\setminus\mathcal{G}} f(p^2)\,\mathrm{d}p + \int_{\mathcal{G}} f(p^2)\,\mathrm{d}p \leq \frac{4\pi^2}{\ell^2}\sum_{p\in(2\pi/\ell)\mathbb{Z}^2} f(p^2) + \int_{\mathcal{G}} f(p^2)\,\mathrm{d}p. \tag{3.3.7}$$

See figure 3.3.1 for an illustration. Then we estimate the integral over $\mathcal{G}$ by four times the

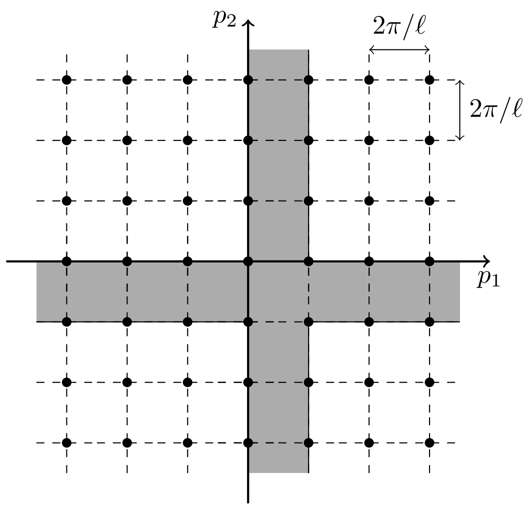

Figure 3.3.1: Illustration of the method of proof of Lemma 9. For the upper bound we use the points that do not lie on a coordinate axis, while for the lower bound we estimate the sum over all points by the integral over the plane without the gray region.

integral over the strip $\{0 < p_1 < 2\pi/\ell \text{ and } p_2 > 0\}$:

$$\int_{\mathcal{G}} f(p^2)\,\mathrm{d}p \le 4 \int_0^{2\pi/\ell} \int_0^\infty f(p_1^2 + p_2^2)\,\mathrm{d}p_2\,\mathrm{d}p_1$$
$$\le \frac{8\pi}{\ell} \int_0^\infty f(p_2^2)\,\mathrm{d}p_2 = \frac{4}{\ell} \int_{\mathbb{R}^2} \frac{f(p^2)}{|p|}\,\mathrm{d}p. \tag{3.3.8}$$

Combining the two previous estimates, we have

$$\sum_{p \in (2\pi/\ell)\mathbb{Z}^2} f(p^2) \ge \frac{\ell^2}{4\pi^2} \int_{\mathbb{R}^2} \left(1 - \frac{4}{\ell|p|}\right) f(p^2)\,\mathrm{d}p. \tag{3.3.9}$$

□

As mentioned in Section 1.2, the definition of the scattering length makes sense for an infinitely ranged potential as well. In that case, (1.2.12) is replaced by

$$\frac{2\pi}{\ln(R/a_R)} = \int_{B_R} \left(|\nabla g_0|^2 + \frac{v}{2}|g_0|^2 \right), \tag{3.3.10}$$

where a_R is the scattering length for the potential with cutoff at R and we already inserted g_0, the solution to (1.2.13), on the right-hand side. It is known from [52, Appendix A] that $a_R \to a$ in a monotonically increasing way as $R \to \infty$, where a is the scattering length of the infinitely ranged potential. This implies in particular that

$$\frac{1}{\ln(R/a_R)} \le \frac{1}{\ln(R/a)}. \tag{3.3.11}$$

For the purpose of proving an upper bound on the free energy, the above inequality will turn out to be useful. In the following, we will work with a potential that satisfies the assumptions of the theorem, i.e., it is nonnegative, possibly infinitely ranged and has a finite scattering length. We recall that in this case (1.2.15) holds, which we will use to estimate terms containing the tail of the potential.

Lemma 10 (Properties of the scattering solution)**.** *Let g_0 be the solution to the zero-energy scattering equation* (1.2.13) *with boundary condition $g_0(R) = 1$. Then the following holds:*

1. *For all $0 < r \le R$*
$$g_0(r) \ge \frac{\ln(r/a_R)}{\ln(R/a_R)}. \tag{3.3.12}$$
2. *The scattering solution g_0 is a monotonically nondecreasing function of r.*

3. *The integral of the derivative of* g_0 *satisfies the bound*

$$\int_{B_R} g_0'(|x|)\,\mathrm{d}x \le \frac{2\pi R}{\ln(R/a_R)}. \tag{3.3.13}$$

Proof. For the proof of the first two properties see [52, proof of Lemma A.1]. For the third one note that since g_0 is a radial function we can just do integration by parts in the radial variable and use that g_0 is always larger than the asymptotic solution. We have

$$\begin{aligned}\int_0^R r g_0'(r)\,\mathrm{d}r &= R g_0(R) - \int_0^R g_0(r)\,\mathrm{d}r \le R - \int_{a_R}^R \frac{\ln(r/a_R)}{\ln(R/a_R)}\,\mathrm{d}r \\ &= R - \frac{1}{\ln(R/a_R)}(R\ln(R/a_R) - R + a_R) = \frac{R - a_R}{\ln(R/a_R)} \\ &\le \frac{R}{\ln(R/a_R)}.\end{aligned} \tag{3.3.14}$$

Note that for $r < a_R$ in the first inequality above we have estimated $g_0(r) \ge 0$. Since the angular integration only gives a factor of 2π, we arrive at the result. □

The last tool we require is a variational formulation of the free energy. For the purpose of proving an upper bound this will turn out to be very useful as we can insert a suitable trial state into the functional. We define the free energy functional first in the canonical setting, then in the grand canonical setting and lastly prove that their thermodynamic limit yields the same free energy. The canonical free energy in finite volume is defined by

$$F_{\mathrm{c}}(\beta, N, L) = \inf_{\Gamma} \left\{ \mathrm{Tr}_{\mathcal{H}_N} H_N \Gamma - \beta^{-1} S(\Gamma) \right\}, \tag{3.3.15}$$

where the infimum is taken over density matrices Γ with N particles. Here, $S(\Gamma)$ is the von Neumann entropy defined by

$$S(\Gamma) = -\,\mathrm{Tr}_{\mathcal{H}_N} \Gamma \ln \Gamma. \tag{3.3.16}$$

On the other hand, the grand canonical free energy in finite volume is defined by

$$F_{\mathrm{gc}}(\beta, N, L) = \inf_{\Gamma} \left\{ \mathrm{Tr}_{\mathcal{F}} \mathbb{H}\Gamma - \beta^{-1} S(\Gamma) \right\}, \tag{3.3.17}$$

where the infimum is taken over density matrices Γ with expected number of particles N and $\mathbb{H}$ is the Hamiltonian on bosonic Fock space, $\mathbb{H} = \bigoplus_{N=0}^{\infty} H_N$. In this expression, $H_0 = 0$, $H_1 = -\Delta$ and H_N as defined in (1.2.1) for $N \ge 2$. Note the slight abuse of notation for the entropy term in (3.3.17): For a state Γ on Fock space it is understood that the trace in $S(\Gamma)$ is also taken on the Fock space $\mathcal{F}$, but we use the same symbol for both entropies. For both the definitions of the free energy in finite volume we can take the thermodynamic limit to obtain the free energy per unit volume as a function of the inverse temperature β and the density ρ

$$f_{\mathrm{c}}(\beta,\rho) = \lim_{\substack{N,L\to\infty \\ N/L^2=\rho}} \frac{F_{\mathrm{c}}(\beta,N,L)}{L^2}, \qquad f_{\mathrm{gc}}(\beta,\rho) = \lim_{\substack{N,L\to\infty \\ N/L^2=\rho}} \frac{F_{\mathrm{gc}}(\beta,N,L)}{L^2}. \tag{3.3.18}$$

Note that by the Gibbs variational principle the canonical free energy per unit volume is equal to the free energy defined in (1.2.4), as can be seen by inserting the minimizing Gibbs state $\Gamma = \mathrm{e}^{-\beta H_N} / \operatorname{Tr}_{\mathcal{H}_N} \mathrm{e}^{-\beta H_N}$ into the canonical free energy functional.

Lemma 11. *We have equality of the canonical and the grand canonical free energy per unit volume in the thermodynamic limit:*

$$f_{\mathrm{c}}(\beta,\rho) = f_{\mathrm{gc}}(\beta,\rho). \tag{3.3.19}$$

In particular, they are both equal to $f(\beta,\rho)$ defined in (1.2.4).

Proof. First of all, we trivially have $f_{\mathrm{gc}}(\beta,\rho) \leq f_{\mathrm{c}}(\beta,\rho)$, since the set which we have to take the infimum of in f_{c} is a subset of the one for f_{gc}. Denote $\mathcal{F}^{\beta,L}(\Gamma)$ the grand canonical free energy functional (i.e., the right-hand side of (3.3.17) without the infimum) and further introduce the grand canonical pressure functional in finite volume

$$-L^2 \mathcal{P}_L^{\beta,\mu}(\Gamma) = \operatorname{Tr}_{\mathcal{F}}(\mathbb{H} - \mu\mathbb{N})\Gamma - \beta^{-1} S(\Gamma), \tag{3.3.20}$$

where $\mathbb{N}$ is the grand canonical particle number operator on Fock space and $\mu \in \mathbb{R}$ is the chemical potential. Maximizing this functional over all density matrices Γ, we obtain the grand canonical pressure in finite volume

$$P_L(\beta,\mu) = \sup_{\Gamma} \mathcal{P}_L^{\beta,\mu}(\Gamma) \tag{3.3.21}$$

and, finally, the thermodynamic pressure is defined by

$$p(\beta,\mu) = \lim_{L\to\infty} P_L(\beta,\mu). \tag{3.3.22}$$

Now we can relate our definition of the grand canonical free energy to the pressure. Let

$\mu \in \mathbb{R}$ and write

$$\begin{aligned} f_{\mathrm{gc}}(\beta,\rho) &= \lim_{L\to\infty} L^{-2} \inf_{\Gamma,\langle\mathbb{N}\rangle_\Gamma=\rho L^2} \mathcal{F}^{\beta,L}(\Gamma) \\ &= \lim_{L\to\infty} L^{-2} \inf_{\Gamma,\langle\mathbb{N}\rangle_\Gamma=\rho L^2} \left(\mathrm{Tr}_{\mathcal{F}}(\mathbb{H}-\mu\mathbb{N})\Gamma - \beta^{-1}S(\Gamma) + \mu\rho L^2\right) \\ &\geq \lim_{L\to\infty} L^{-2} \inf_{\Gamma} \left(-L^2\mathcal{P}_L^{\beta,\mu}(\Gamma) + \mu\rho L^2\right) = \mu\rho - \lim_{L\to\infty}\sup_{\Gamma} \mathcal{P}_L^{\beta,\mu}(\Gamma) = \mu\rho - p(\beta,\mu). \end{aligned} \tag{3.3.23}$$

In the inequality above we relaxed the condition on the expectation of the particle number operator and thus have obtained the pressure. This holds for every μ and we can take the supremum over all μ of the right-hand side above. It is a well-known fact (see, e.g., Theorem 3.5.8 in [66]) that the canonical free energy is the Legendre transform of the pressure and thus we have shown

$$f_{\mathrm{gc}}(\beta,\rho) \geq \sup_{\mu}\left(\mu\rho - p(\beta,\mu)\right) = f_{\mathrm{c}}(\beta,\rho) \tag{3.3.24}$$

and consequently $f_{\mathrm{c}}(\beta,\rho) = f_{\mathrm{gc}}(\beta,\rho)$. □

3.4 Changing boundary conditions

In this subsection, we present a method that relates Hamiltonians with different boundary conditions. We need some arguments from [65] which we repeat here for the reader's convenience. Let us put the center of the box at the origin and denote the size of the box via subscript:

$$\Lambda_L = \left\{x = (x^{(1)}, x^{(2)}) \in \mathbb{R}^2 : -\frac{L}{2} < x^{(i)} < \frac{L}{2}, i = 1,2\right\} \tag{3.4.1}$$

We define a reflection mapping from Λ_{3L} to Λ_L as follows. Geometrically speaking, for $x \in \Lambda_{3L}\backslash\Lambda_L$ we associate to it the point x^{R} obtained via reflection along the edge (or edges) of Λ_L such that $x^{\mathrm{R}} \in \Lambda_L$ and for $x \in \Lambda_L$, we set $x^{\mathrm{R}} = x$. See figure 3.4.2 for an illustration. More formally, we note that for every $x \in \Lambda_{3L}\backslash\overline{\Lambda_L}$ there exists a unique[1] $\ell_x \in \mathbb{R}^2$ that is of the form $\ell_x = (n_x^{(1)}L, n_x^{(2)}L)$ with $n_x^{(i)} \in \{0, \pm 1\}$ and satisfies $x + \ell_x \in \Lambda_L$. We then define

$$x^{\mathrm{R}} = \left(-n_x^{(1)}L + (-1)^{n_x^{(1)}}x^{(1)}, -n_x^{(2)}L + (-1)^{n_x^{(2)}}x^{(2)}\right). \tag{3.4.2}$$

[1]Note that the boundary of Λ_L has to be excluded in order to make ℓ_x unique. Since the set has zero measure in Λ_{3L}, this is of no consequence, however.

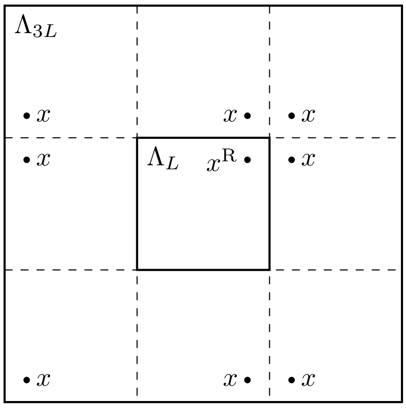

Figure 3.4.2: Illustration of the reflection mapping: Each point x has the point x^{R} as image.

For wave functions $\psi \in \mathcal{H}_N(\Lambda_L)$ we define the reflected wave function on the larger box $\psi^{\mathrm{R}} \in \mathcal{H}_N(\Lambda_{3L})$ by

$$\psi^{\mathrm{R}}(x_1, \ldots, x_N) = \psi(x_1^{\mathrm{R}}, \ldots, x_N^{\mathrm{R}}). \tag{3.4.3}$$

Finally, for $0 < b < L/2$, we introduce a cutoff function h on the real line with the following properties.

1. h is real, even and continuously differentiable
2. $h(x) = 0$ for $|x| > L/2 + b$
3. $h(x) = 1$ for $|x| < L/2 - b$
4. $|h(x)|^2 + |h(-x - L)|^2 = 1$ for $-L/2 - b \leq x \leq -L/2$
5. $|h'(x)|^2 \leq 1/b^2$, $|h(x)|^2 \leq 1$ for all $x \in \mathbb{R}$

Condition 4. is nothing else but the fact that $y \mapsto 1/2 - |h(y - L/2)|^2$ is antisymmetric on $[-b, b]$. For points in the plane, $x = (x^{(1)}, x^{(2)}) \in \mathbb{R}^2$, we set by abuse of notation $h(x) = h(x^{(1)})h(x^{(2)})$ and lastly define

$$\begin{aligned} &V : \mathcal{H}_N(\Lambda_L) \to \mathcal{H}_N(\Lambda_{L+2b}), \\ &\psi(x_1, \ldots, x_N) \mapsto (V\psi)(x_1, \ldots, x_N) = \psi^{\mathrm{R}}(x_1, \ldots, x_N) \prod_{i=1}^{N} h(x_i). \end{aligned} \tag{3.4.4}$$

Lemma 12 (Lemma 2.1.12 from [65])**.** *The mapping V introduced in* (3.4.4) *is an isometry.*

Proof. We need to show for all ϕ and ψ that

$$\langle V\phi, V\psi\rangle_{\mathcal{H}_N(\Lambda_{L+2b})} = \langle \phi, \psi\rangle_{\mathcal{H}_N(\Lambda_L)} \,. \tag{3.4.5}$$

The left-hand side is given explicitly by

$$\begin{aligned}\langle V\phi, V\psi\rangle_{\mathcal{H}_N(\Lambda_{L+2b})} &= \int_{\Lambda_{L+2b}^N} (\overline{V\phi})(x_1,\dots,x_N)(V\psi)(x_1,\dots,x_N)\,\mathrm{d}X_N \\ &= \int_{[-L/2-b,L/2+b]^{2N}} \overline{\phi^{\mathrm{R}}}(x_1,\dots,x_N)\psi^{\mathrm{R}}(x_1,\dots,x_N)\prod_{i=1}^N |h(x_i)|^2\,\mathrm{d}X_N. \end{aligned} \tag{3.4.6}$$

Recall that by definition of h we have for $x \in \mathbb{R}^2$ that $h(x) = h(x^{(1)})h(x^{(2)})$ and this means the last part of the integrand (without ϕ and ψ) factorizes completely. Thus we consider the integral over one component of one coordinate only. Say we fix $(x_2,\dots,x_N)$ and additionally the second component of x_1, such that the integrand is a function of $x_1^{(1)}$ only. Then we consider

$$F(Y) = \int_{-L/2-b}^{L/2+b} \overline{\phi^{\mathrm{R}}}(t,Y)\psi^{\mathrm{R}}(t,Y)|h(t)|^2\,\mathrm{d}t, \tag{3.4.7}$$

where we introduced the shorthand $Y = (x_1^{(2)}, x_2,\dots,x_N)$. By construction, we have

$$\int F(Y)\prod_{y\in Y}|h(y)|^2\,\mathrm{d}Y = \langle V\phi, V\psi\rangle\,. \tag{3.4.8}$$

The one-dimensional integral in $F(Y)$ can now be evaluated. We have

$$\begin{aligned} F(Y) &= \int_{-L/2-b}^{L/2+b} \overline{\phi}(t^{\mathrm{R}},Y^{\mathrm{R}})\psi(t^{\mathrm{R}},Y^{\mathrm{R}})|h(t)|^2\,\mathrm{d}t \\ &= \left[\int_{-L/2-b}^{-L/2} + \int_{-L/2}^{-L/2+b} + \int_{-L/2+b}^{L/2-b} + \int_{L/2-b}^{L/2} + \int_{L/2}^{L/2+b}\right]\overline{\phi}(t^{\mathrm{R}},Y^{\mathrm{R}})\psi(t^{\mathrm{R}},Y^{\mathrm{R}})|h(t)|^2\,\mathrm{d}t \\ &= S_E^{(1)} + S_I^{(1)} + I + S_I^{(2)} + S_E^{(2)}. \end{aligned} \tag{3.4.9}$$

We consider each term in the sum above separately. First, we note that in the region $[-L/2, L/2]$ (so for the three middle terms) the reflection mapping acts as an identity, such that $t^{\mathrm{R}} = t$ there. Second, the function h is equal to one in $[-L/2+b, L/2-b]$ and thus

$$I = \int_{-L/2+b}^{L/2-b} \overline{\phi}(t,Y^{\mathrm{R}})\psi(t,Y^{\mathrm{R}})\,\mathrm{d}t. \tag{3.4.10}$$

Now we consider the term $S_E^{(1)}$. We want to perform a coordinate transformation such that we integrate over $[-L/2, -L/2+b]$ instead of $[-L/2-b, -L/2]$ (which is the integration region of $S_I^{(1)}$). This is done exactly via the reflection mapping defined above and hence we obtain for the sum of $S_E^{(1)}$ and $S_I^{(1)}$

$$\begin{aligned} S_E^{(1)} + S_I^{(1)} &= \int_{-L/2-b}^{-L/2} \overline{\phi}(t^{\mathrm{R}}, Y^{\mathrm{R}})\psi(t^{\mathrm{R}}, Y^{\mathrm{R}})|h(t)|^2 \,\mathrm{d}t + \int_{-L/2}^{-L/2+b} \overline{\phi}(t, Y^{\mathrm{R}})\psi(t, Y^{\mathrm{R}})|h(t)|^2 \,\mathrm{d}t \\ &= \int_{-L/2}^{-L/2+b} \overline{\phi}(t, Y^{\mathrm{R}})\psi(t, Y^{\mathrm{R}})|h(t^{\mathrm{R}})|^2 \,\mathrm{d}t + \int_{-L/2}^{-L/2+b} \overline{\phi}(t, Y^{\mathrm{R}})\psi(t, Y^{\mathrm{R}})|h(t)|^2 \,\mathrm{d}t \\ &= \int_{-L/2}^{-L/2+b} \overline{\phi}(t, Y^{\mathrm{R}})\psi(t, Y^{\mathrm{R}})(|h(t^{\mathrm{R}})|^2 + |h(t)|^2) \,\mathrm{d}t \\ &= \int_{-L/2}^{-L/2+b} \overline{\phi}(t, Y^{\mathrm{R}})\psi(t, Y^{\mathrm{R}}) \,\mathrm{d}t. \end{aligned} \tag{3.4.11}$$

The last equality follows because of the antisymmetry of h specified in condition 4. We proceed analogously for the term $S_I^{(2)} + S_E^{(2)}$ and obtain

$$F(Y) = \int_{-L/2}^{L/2} \overline{\phi}(t, Y^{\mathrm{R}})\psi(t, Y^{\mathrm{R}}) \,\mathrm{d}t. \tag{3.4.12}$$

Repeating this procedure for all other coordinates, we arrive at the result. □

Lemma 13. *Assume that the interaction v is nonnegative. Then define the Dirichlet and Neumann Hamiltonians on the boxes of size $L+2b$ and L, respectively, by*

$$\begin{aligned} H_{N,\Lambda_{L+2b}}^{Dirichlet} &= -\sum_{i=1}^{N} \Delta_{i,L+2b}^{Dirichlet} + \sum_{i<j}^{N} v(d(x_i, x_j)), \\ H_{N,\Lambda_L}^{Neumann} &= -\sum_{i=1}^{N} \Delta_{i,L}^{Neumann} + \sum_{i<j}^{N} v(d(x_i, x_j)), \end{aligned} \tag{3.4.13}$$

where the Laplacians are to be taken with the indicated boundary conditions and sizes of the boxes. Then for ψ in the domain of $H_{N,\Lambda_L}^{Neumann}$ we have the estimate

$$\begin{aligned} \langle V\psi, H_{N,\Lambda_{L+2b}}^{Dirichlet} V\psi\rangle \leq \langle \psi, H_{N,\Lambda_L}^{Neumann}\psi\rangle + \frac{4N}{b^2}\|\psi\|^2 \\ + \frac{1}{2}\int_{\mathcal{B}_L^b} v(d(x,y))\rho_\psi^{(2)}(x^{\mathrm{R}}, y^{\mathrm{R}})h(x)h(y) \,\mathrm{d}x\,\mathrm{d}y. \end{aligned} \tag{3.4.14}$$

Here, $\mathcal{B}_L^b = \Lambda_{L+2b}^2 \backslash \Lambda_L^2$ and $\rho_\psi^{(2)}$ denotes the two-particle density of ψ defined by

$$\rho_\psi^{(2)}(x_1, x_2) = N(N-1) \int_{\Lambda_L^{N-2}} |\psi(X_N)|^2 \,\mathrm{d}x_3 \cdots \mathrm{d}x_N. \tag{3.4.15}$$

Proof. Let ψ be a bosonic wave function on Λ_L obeying Neumann boundary conditions. The left-hand side is then given by

$$\begin{aligned}\langle V\psi, H_{N,\Lambda_{L+2b}}^{\text{Dirichlet}} V\psi\rangle = &\int_{\Lambda_{L+2b}^N} |(\nabla\psi^{\mathrm{R}}(X_N))h(X_N) + \psi^{\mathrm{R}}(X_N)\nabla h(X_N)|^2 \,\mathrm{d}X_N \\ &+ \sum_{i<j} \int_{\Lambda_{L+2b}^N} v(d(x_i, x_j))|(V\psi)(X_N)|^2 \,\mathrm{d}X_N.\end{aligned} \tag{3.4.16}$$

By expanding the square in the first term we obtain three terms. The first one is

$$\int_{\Lambda_{L+2b}^N} |\nabla\psi^{\mathrm{R}}(X_N)|^2 |h(X_N)|^2 \,\mathrm{d}X_N = \int_{\Lambda_L^N} |\nabla\psi(X_N)|^2 \,\mathrm{d}X_N, \tag{3.4.17}$$

where we applied Lemma 12 to $\nabla\psi$ to change the integration region and eliminate the factors of $|h|^2$. The second term is given by

$$\int_{\Lambda_{L+2b}^N} |\psi^{\mathrm{R}}(X_N)|^2 |\nabla h(X_N)|^2 \,\mathrm{d}X_N. \tag{3.4.18}$$

The square of the gradient is a sum of $2N$ terms. Consider the first one of these where the gradient acts on the $x_1^{(1)}$ coordinate and denote again $Y = (x_1^{(2)}, x_2, \dots, x_N)$. The derivative of h in the first variable (call it t) can be estimated using condition 5 in the definition of h and the remaining factors of h will be used again to change the region of integration in the Y variables:

$$\begin{aligned}&\int_{[-L/2-b,L/2+b]^{2N-1}} \int_{-L/2-b}^{L/2+b} |\psi^{\mathrm{R}}(t, Y)|^2 |h'(t)|^2 \,\mathrm{d}t \prod_{y\in Y} |h(y)|^2 \,\mathrm{d}Y \\ &= \int_{[-L/2-b,L/2+b]^{2N-1}} \int_{-L/2}^{L/2} |\psi(t, Y^{\mathrm{R}})|^2 \left(|h'(t)|^2 + |h'(t^{\mathrm{R}})|^2\right) \mathrm{d}t \prod_{y\in Y} |h(y)|^2 \,\mathrm{d}Y \\ &\le \frac{2}{b^2} \int_{[-L/2-b,L/2+b]^{2N-1}} \int_{-L/2}^{L/2} |\psi(t, Y^{\mathrm{R}})|^2 \,\mathrm{d}t \prod_{y\in Y} |h(y)|^2 \,\mathrm{d}Y \\ &= \frac{2}{b^2} \int_{\Lambda_L^N} |\psi(X_N)|^2 \,\mathrm{d}X_N = \frac{2}{b^2}\|\psi\|^2.\end{aligned} \tag{3.4.19}$$

We apply this bound to every term in the sum and obtain the upper bound $4N\|\psi\|^2/b^2$ for (3.4.18). The third and last term is the mixed term appearing in the square of the gradient above. It can be written as

$$\frac{1}{2}\int_{\Lambda_{L+2b}^N} \nabla|\psi^{\mathrm{R}}(X_N)|^2 \cdot \nabla|h(X_N)|^2 \,\mathrm{d}X_N. \tag{3.4.20}$$

Since the gradient of h vanishes on $[-L/2+b, L/2-b]$ in every coordinate, the integral is only over the two remaining end intervals. We want to argue now that both of these terms vanish due to the symmetry properties of the integrand. One of the terms that appear in the integral above is

$$\frac{1}{2}\int_{-L/2-b}^{-L/2+b} \left(\frac{\partial}{\partial x_1^{(1)}}|\psi^{\mathrm{R}}(X_N)|^2\right)\left(\frac{\partial}{\partial x_1^{(1)}}|h(X_N)|^2\right) \mathrm{d}x_1^{(1)}. \tag{3.4.21}$$

Now it is easy to see that since $|\psi^{\mathrm{R}}|^2$ is an even function of $x_1^{(1)}$ on the interval $[-L/2-b, -L/2+b]$ (with respect to $-L/2$, by definition of the reflection mapping), the derivative in that direction will be an odd function. Similarly, since $|h|^2 - 1/2$ is an odd function on $[-L/2-b, -L/2+b]$ (with respect to $-L/2$), the derivative will be an even function. Consequently, the integral over the product of an odd with an even function must vanish. This holds true for every term in the sum and thus the third term is identically zero.

Finally, we consider the term involving the interaction. Note that $v(d(x,y)) = v(d(x^{\mathrm{R}}, y^{\mathrm{R}}))$ whenever x and y both lie within Λ_L, which implies

$$\int_{\Lambda_{L+2b}^2} \Big(v(d(x,y)) - v(d(x^{\mathrm{R}}, y^{\mathrm{R}}))\Big) f(x,y)\,\mathrm{d}x\,\mathrm{d}y = \int_{\mathcal{B}_L^b} \Big(v(d(x,y)) - v(d(x^{\mathrm{R}}, y^{\mathrm{R}}))\Big) f(x,y)\,\mathrm{d}x\,\mathrm{d}y \tag{3.4.22}$$

for some function f and where we defined $\mathcal{B}_L^b = \Lambda_{L+2b}^2 \backslash \Lambda_L^2$ to be the set of (x,y) in Λ_{L+2b}^2 with those points removed that lie both within Λ_L. We have

$$\begin{aligned}\sum_{i<j}^{N}\int_{\Lambda_{L+2b}^N} v(d(x_i,x_j))|(V\psi)(X_N)|^2\,\mathrm{d}X_N &= \sum_{i<j}^{N}\int_{\Lambda_L^N} v(d(x_i,x_j))|\psi(X_N)|^2\,\mathrm{d}X_N \\ &+ \sum_{i<j}^{N}\int_{\Lambda_{L+2b}^N} \Big(v(d(x_i,x_j)) - v(d(x_i^{\mathrm{R}}, x_j^{\mathrm{R}}))\Big)|(V\psi)(X_N)|^2\,\mathrm{d}X_N,\end{aligned} \tag{3.4.23}$$

where we used Lemma 12 to obtain the first term on the right-hand side. We denote in the following calculation by $\hat{X}_{N-2}^{i,j}$ the $(N-2)$-tuple $(x_1, \ldots, x_N)$ where x_i and x_j are missing.

By the symmetry of ψ and using (3.4.22), we can rewrite the second term on the right-hand side above as

$$
\begin{aligned}
&\sum_{i<j}^{N} \int_{\Lambda_{L+2b}^{N}} \Big(v(d(x_i,x_j)) - v(d(x_i^{\mathrm{R}},x_j^{\mathrm{R}}))\Big) |(V\psi)(X_N)|^2 \,\mathrm{d}X_N \\
&= \sum_{i<j}^{N} \int_{\Lambda_{L+2b}^{2}} \Big(v(d(x_i,x_j)) - v(d(x_i^{\mathrm{R}},x_j^{\mathrm{R}}))\Big)\left(\int_{\Lambda_{L+2b}^{N-2}} |(V\psi)(X_N)|^2 \,\mathrm{d}\hat{X}_{N-2}^{i,j}\right) \mathrm{d}x_i \,\mathrm{d}x_j \\
&= \frac{N(N-1)}{2} \int_{\mathcal{B}_L^b} \Big(v(d(x_1,x_2)) - v(d(x_1^{\mathrm{R}},x_2^{\mathrm{R}}))\Big)\left(\int_{\Lambda_{L+2b}^{N-2}} |(V\psi)(X_N)|^2 \,\mathrm{d}\hat{X}_{N-2}^{1,2}\right) \mathrm{d}x_1 \,\mathrm{d}x_2 \\
&= \frac{1}{2} \int_{\mathcal{B}_L^b} \Big(v(d(x,y)) - v(d(x^{\mathrm{R}},y^{\mathrm{R}}))\Big) \rho_{V\psi}^{(2)}(x,y) \,\mathrm{d}x \,\mathrm{d}y \\
&\leq \frac{1}{2} \int_{\mathcal{B}_L^b} v(d(x,y)) \rho_{V\psi}^{(2)}(x,y) \,\mathrm{d}x \,\mathrm{d}y \\
&= \frac{1}{2} \int_{\mathcal{B}_L^b} v(d(x,y)) \rho_{\psi}^{(2)}(x^{\mathrm{R}},y^{\mathrm{R}}) h(x) h(y) \,\mathrm{d}x \,\mathrm{d}y.
\end{aligned} \tag{3.4.24}
$$

In the calculation, we recognized the two-particle density $\rho_{V\psi}^{(2)}$ of $V\psi$, in the inequality we simply threw away the negative term and then used once again Lemma 12 to obtain $\rho_{\psi}^{(2)}$. The first term on the right-hand side of (3.4.23) constitutes the interaction part of $\langle\psi, H_{N,\Lambda_L}^{\mathrm{Neumann}}\psi\rangle$, while using the calculation in (3.4.24) for the second term leads directly to the term in the second line of (3.4.14). Combining the estimates for the gradient and the interaction terms, we obtain the result. □

Remark. If the interaction were decreasing, the statement of Lemma 13 would be different: We would not obtain the term in the second line of (3.4.14). Instead, when starting from the left-hand side of (3.4.23), we simply use that the reflection mapping $x \mapsto x^{\mathrm{R}}$ is a contraction and apply Lemma 12 to obtain

$$
\begin{aligned}
\sum_{i<j}^{N} \int_{\Lambda_{L+2b}^{N}} v(d(x_i,x_j)) |(V\psi)(X_N)|^2 \,\mathrm{d}X_N &\leq \sum_{i<j}^{N} \int_{\Lambda_{L+2b}^{N}} v(d(x_i^{\mathrm{R}},x_j^{\mathrm{R}})) |(V\psi)(X_N)|^2 \,\mathrm{d}X_N \\
&= \sum_{i<j}^{N} \int_{\Lambda_{L}^{N}} v(d(x_i,x_j)) |\psi(X_N)|^2 \,\mathrm{d}X_N.
\end{aligned} \tag{3.4.25}
$$

Below, in the application of Lemma 13, we will have more information about ψ and its two-particle density $\rho_{\psi}^{(2)}$ and are able to estimate the term on the right-hand side in (3.4.24). It can then be seen that thanks to the small volume of $\mathcal{B}_L^b$ the whole term is small.

Furthermore, we can replace Neumann boundary conditions by periodic boundary conditions in Lemma 13 since we have

$$\langle \psi, H^{\text{Neumann}}_{N,\Lambda_L} \psi \rangle \leq \langle \psi, H^{\text{periodic}}_{N,\Lambda_L} \psi \rangle \tag{3.4.26}$$

for any wave function ψ obeying Neumann boundary conditions, see [65, Proof of Proposition 2.3.7].

3.5 Box method and strategy of proof

We now explain in more detail the strategy we use to prove Theorem 3. As is appropriate for an upper bound, we will construct a trial state that we insert into the grand canonical free energy functional. Consider a partition of the square of size L into $(L/\ell)^2$ smaller boxes of size ℓ, and define the trial state Γ to be a tensor product of identical (up to translation) states Γ^i that only live on each small box and obey Dirichlet boundary conditions there, i.e.,

$$\Gamma = \bigotimes_i \Gamma^i. \tag{3.5.1}$$

Strictly speaking, we can only partition the square into $\lfloor L^2/\ell^2 \rfloor$ (the largest integer smaller than L^2/ℓ^2) boxes and will have some space left over at the boundary of the box. As we take the limit $L \to \infty$ this effect will become negligible.

By the variational principle we then have

$$f(\beta, \rho) = \lim_{L\to\infty} L^{-2} F_{\text{gc}}(\beta, \rho L^2, L) \leq \lim_{L\to\infty} L^{-2} \mathcal{F}^{\beta,L}(\Gamma) \tag{3.5.2}$$

under the condition that Γ has to have $N = \rho L^2$ particles. Since the states Γ^i are identical up to translation, we can evaluate $\mathcal{F}^{\beta,L}(\Gamma)$ further as

$$\mathcal{F}^{\beta,L}(\Gamma) = \frac{L^2}{\ell^2} \mathcal{F}^{\beta,\ell}(\Gamma^1) + \text{Tr}_{\mathcal{F}} \left[\bigoplus_{N\geq 2} \sum_{i<j}^{N} v(d(x_i, x_j)) \mathbb{1}_{i,j} \bigotimes_k \Gamma^k \right], \tag{3.5.3}$$

where the second term is due to the infinite range of the potential and $\mathbb{1}_{i,j}$ is the characteristic function of two particles being in different boxes. This term can be estimated simply assuming we have a bound on the two-particle density of Γ:

$$\begin{aligned} \text{Tr}_{\mathcal{F}} \left[\bigoplus_{N\geq 2} \sum_{i<j}^{N} v(d(x_i, x_j)) \mathbb{1}_{i,j} \bigotimes_k \Gamma^k \right] &\lesssim L^2 \rho^2 \int_{|x|>R} v(|x|) \, \mathrm{d}x \\ &\leq \frac{L^2 \rho^2}{\ln^2(R/a)} \int_{|x|>a} v(|x|) \ln^2(|x|/a) \, \mathrm{d}x. \end{aligned} \tag{3.5.4}$$

Using (1.2.15), we have the bound

$$\text{r.h.s. of (3.5.4)} \leq \frac{CL^2\rho^2}{\ln^2(R/a)} \tag{3.5.5}$$

for a constant $C > 0$.

Let the Dirichlet trial state be given as $\Gamma^1 = V^*\Gamma^1_P V$ for a periodic trial state density matrix $\Gamma^1_P = \sum_\alpha \nu_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$, where V is as defined in (3.4.4). Note that Γ^1 is defined on a box of linear size ℓ and Γ^1_P is defined on a box of linear size $\ell - 2b$, which requires to plug in $L = \ell - 2b$ into the definition of V. Then we apply Lemma 13 (and the remark (3.4.26)) to obtain

$$\begin{aligned}
&\mathrm{Tr}_{\mathcal{F}}\, \mathbb{H}^{\mathrm{Dir}}\Gamma^1 = \mathrm{Tr}_{\mathcal{F}}\left(\mathbb{H}^{\mathrm{Dir}} V^*\Gamma^1_P V\right) = \mathrm{Tr}_{\mathcal{F}}\left(\mathbb{H}^{\mathrm{Dir}} V^* \sum_\alpha \nu_\alpha |\phi_\alpha\rangle\langle\phi_\alpha| V\right) \\
&= \sum_\alpha \nu_\alpha \langle V\phi_\alpha, H^{\mathrm{Dir}}_{N_\alpha} V\phi_\alpha\rangle \\
&\leq \sum_\alpha \nu_\alpha \Bigg(\langle\phi_\alpha, H^{\mathrm{per}}_{N_\alpha}\phi_\alpha\rangle + \frac{4N_\alpha}{b^2}\|\phi_\alpha\|^2 \\
&\qquad + \frac{1}{2}\int_{\mathcal{B}^b_{\ell-2b}} v(d(x,y))\rho^{(2)}_{\phi_\alpha}(x^{\mathrm{R}}, y^{\mathrm{R}})h(x)h(y)\,\mathrm{d}x\,\mathrm{d}y\Bigg) \\
&= \mathrm{Tr}_{\mathcal{F}}\, \mathbb{H}^{\mathrm{per}}\Gamma^1_P + \frac{4}{b^2}\rho\ell^2 + \frac{1}{2}\sum_\alpha \nu_\alpha \int_{\mathcal{B}^b_{\ell-2b}} v(d(x,y))\rho^{(2)}_{\phi_\alpha}(x^{\mathrm{R}}, y^{\mathrm{R}})h(x)h(y)\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned}\tag{3.5.6}$$

We use further that the von Neumann entropy is invariant under isometries (i.e., $S(\rho) = S(V^*\rho V)$ for an isometry V) to obtain

$$\begin{aligned}
f(\beta,\rho) \leq{}& \ell^{-2}\mathcal{F}^{\beta,\ell-2b}(\Gamma^1_P) + \frac{4\rho}{b^2} + \frac{C\rho^2}{\ln^2(R/a)} \\
&+ \frac{1}{2\ell^2}\sum_\alpha \nu_\alpha \int_{\mathcal{B}^b_{\ell-2b}} v(d(x,y))\rho^{(2)}_{\phi_\alpha}(x^{\mathrm{R}}, y^{\mathrm{R}})h(x)h(y)\,\mathrm{d}x\,\mathrm{d}y.
\end{aligned}\tag{3.5.7}$$

We are left with the task of finding an upper bound to the free energy of a periodic trial state which we do in the next section. The trial state that we will use consists of a Gibbs state, a manually tuned quasi-condensate and a product function that adds correlations to the system, see (3.6.1) below.

A small caveat of this method is that the constructed trial state Γ is not symmetrical under exchange of the particles as would be appropriate for bosons. This is not a problem though, as the following example shows. Consider two one-particle wave functions ϕ_1 and ϕ_2 that have disjoint support, i.e., we have $\phi_1\phi_2 = 0$. A symmetric state built out of ϕ_1 and ϕ_2 is

$$\psi(x_1, x_2) = \frac{1}{\sqrt{2}} \left(\phi_1(x_1)\phi_2(x_2) + \phi_2(x_1)\phi_1(x_2)\right). \tag{3.5.8}$$

Take O to be a local two-particle observable. This means that $\phi_1 O \phi_2 = \phi_2 O \phi_1 = 0$. Then we have

$$\begin{aligned}\langle\psi|O|\psi\rangle = \frac{1}{2}\Big(&\langle\phi_1\otimes\phi_2|O|\phi_1\otimes\phi_2\rangle + \langle\phi_1\otimes\phi_2|O|\phi_2\otimes\phi_1\rangle \\ &+ \langle\phi_2\otimes\phi_1|O|\phi_1\otimes\phi_2\rangle + \langle\phi_2\otimes\phi_1|O|\phi_2\otimes\phi_1\rangle\Big) \\ = \langle&\phi_1\otimes\phi_2|O|\phi_1\otimes\phi_2\rangle, \end{aligned} \tag{3.5.9}$$

where we used in the calculation that O is symmetric under exchange of coordinates. Thus, it is enough to consider $\phi_1 \otimes \phi_2$ if one is interested in local expectation values of the symmetric state ψ.

3.6 Estimate on finite box for periodic trial state

We now construct a periodic trial state on the box of size $\tilde{\ell} = \ell - 2b$ with expected number of particles $n = \rho\ell^2$ and subsequently give an upper bound on its free energy. For this purpose we present lemmas that estimate the norm, particle number, energy and entropy of the trial state. The basic ingredients we need to build up the trial density matrix are a product function (that introduces correlations), the grand canonical Gibbs state of the non-interacting system and a coherent state operator representing the quasi-condensate. More precisely, our trial state is

$$\Gamma = \sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha \frac{|fD_z\psi_\alpha\rangle\langle fD_z\psi_\alpha|}{\|fD_z\psi_\alpha\|^2}. \tag{3.6.1}$$

where the meaning of the symbols is as follows. The f is an operator on Fock space, the ψ_α and λ_α are the eigenfunctions and eigenvalues of the grand canonical Gibbs state of the non-interacting system and D_z is the coherent state (Weyl) operator for the $p = 0$ mode. More precisely, f is an operator on Fock space that acts in the sector of particle number $k \geq 2$ as

$$f_k = P_k f P_k = \prod_{i<j}^{k} g(d(x_i, x_j))P_k, \tag{3.6.2}$$

where P_k is the projector to particle number k, $g(x) = g_0(x)$ for $0 \leq x \leq R$, $g(x) = 1$ for $x > R$ and g_0 solves (1.2.13) in the sense of distributions on B_R with boundary condition $g_0(R) = 1$. For $k = 0$ or $k = 1$ we define f_k to be the identity operator. The parameter R will be chosen to satisfy the conditions

$$a \ll R \ll \rho^{-1/2}, \tag{3.6.3}$$

i.e., it should be much larger than the scattering length of the potential yet much smaller than the average inter-particle distance. The objects with index α are related to the Gibbs state of the non-interacting system, which we write as

$$\Gamma_G = \sum_{\alpha} \lambda_\alpha |\psi_\alpha\rangle\langle\psi_\alpha|, \tag{3.6.4}$$

where the ψ_α are the (orthonormal) eigenfunctions of the grand canonical Laplacian (i.e., the direct sum of the N-particle Laplacian in every particle number sector) with periodic boundary conditions on the box and λ_α the eigenvalues of the Gibbs state. Explicitly,

$$\lambda_\alpha = \frac{\mathrm{e}^{-\beta(E_\alpha - \mu_0 N_\alpha)}}{\sum_{\alpha'} \mathrm{e}^{-\beta(E_{\alpha'} - \mu_0 N_{\alpha'})}}, \tag{3.6.5}$$

where μ_0 is chosen such that Γ_G has density $\rho_G = n_G/\ell^2$ (which is achieved by inserting $\rho = \rho_G$ into $\mu(\beta, \rho)$ from (1.2.7)) and E_α are the corresponding eigenvalues to ψ_α. For reasons that will become apparent when we estimate the norm $\|f D_z \psi_\alpha\|^2$, we introduce a cutoff on the number of particles in Γ by restricting the sum in (3.6.1) to the set

$$\mathcal{A} = \{\alpha : N_\alpha < \mathcal{N}\}. \tag{3.6.6}$$

Here, N_α is the number of coordinates (particles) of ψ_α and $\mathcal{N}$ is a parameter to be chosen later. In order for the trial state Γ to still have trace one, we need to modify the coefficients λ_α and use instead

$$\tilde{\lambda}_\alpha = \frac{\lambda_\alpha}{\sum_{\alpha' \in \mathcal{A}} \lambda_{\alpha'}}. \tag{3.6.7}$$

This ensures $\mathrm{Tr}_{\mathcal{F}} \Gamma = \sum_{\alpha \in \mathcal{A}} \tilde{\lambda}_\alpha = 1$.

We use the notation a_p and $a_p^\dagger$ for the annihilation and creation operators of a plane wave of momentum p on Fock space. By abuse of notation, we shall use the same symbol for the plane wave expansion of the annihilation and creation operators and we change only the letter of the subscript as long as no confusion arises, i.e.,

$$a_x := \sum_p a_p \frac{\mathrm{e}^{ipx}}{\tilde{\ell}}, \tag{3.6.8}$$

and analogously for $a_x^\dagger$.

Finally, for $z \in \mathbb{C}$, D_z is the coherent state (Weyl) operator for the $p = 0$ mode

$$D_z = \exp\left(z a_0^\dagger - \bar{z} a_0\right). \tag{3.6.9}$$

It acts as a shift operator on the $p = 0$ mode creation/annihilation operators and as identity on the other modes in the momentum space representation,

$$D_z^\dagger a_p D_z = a_p + z\delta_{p,0}. \tag{3.6.10}$$

This implies

$$D_z^\dagger a_x D_z = \sum_p D_z^\dagger a_p D_z \frac{e^{ipx}}{\tilde{\ell}} = \sum_p a_p \frac{e^{ipx}}{\tilde{\ell}} + \frac{z}{\tilde{\ell}}\delta_{p,0} = a_x + \frac{z}{\tilde{\ell}}. \tag{3.6.11}$$

Furthermore, Γ needs to have expected number of particles equal to n to be admissible. This means

$$\begin{aligned}\langle \mathbb{N} \rangle_\Gamma = \mathrm{Tr}_{\mathcal{F}}\, \mathbb{N}\Gamma &= \sum_{\alpha\in\mathcal{A}} \frac{\tilde{\lambda}_\alpha}{\|fD_z\psi_\alpha\|^2} \langle fD_z\psi_\alpha | \mathbb{N} | fD_z\psi_\alpha \rangle \\ &= \sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha (N_\alpha + |z|^2) = \sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha N_\alpha + |z|^2 \overset{!}{=} n. \end{aligned} \tag{3.6.12}$$

The total particle number is given as the sum of particles in the (modified) thermal Gibbs state, $\tilde{n}_G = \sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha N_\alpha$, and particles in the added condensate, $n_0 = |z|^2$, as $n = \tilde{n}_G + n_0$. Therefore, we have the following relation between n_G and $\tilde{n}_G$:

$$n_G = \tilde{n}_G \sum_{\alpha\in\mathcal{A}} \lambda_\alpha + \sum_{\alpha\notin\mathcal{A}} \lambda_\alpha N_\alpha = (n - n_0) \sum_{\alpha\in\mathcal{A}} \lambda_\alpha + \sum_{\alpha\notin\mathcal{A}} \lambda_\alpha N_\alpha. \tag{3.6.13}$$

Below, we will see that approximately $n_G \approx n - n_0$.

We divide the calculation for the upper bound of the free energy of the trial state Γ into four lemmas which we prove separately. We start with an estimate about the norm appearing in the denominator of Γ.

Lemma 14 (Norm estimate)**.** *Independently of $\alpha \in \mathcal{A}$, we have the lower bound*

$$\|fD_z\psi_\alpha\|^2 \geq 1 - \frac{\pi R^2}{2\tilde{\ell}^2}\left(|z|^4 + 4|z|^2\mathcal{N} + 2\mathcal{N}^2\right) =: \frac{1}{B_1}. \tag{3.6.14}$$

Proof. First of all, we observe that the function g is equal to one except in a region of size R (by definition). In other words, we can write

$$g(x)^2 = 1 - \eta(x), \tag{3.6.15}$$

where η has support in a disk of radius R and takes values between zero and one. Thus we have

$$\begin{aligned} \|fD_z\psi_\alpha\|^2 &= \sum_m \int |(D_z\psi_\alpha)_m|^2 \prod_{i<j}^m g(x_i - x_j)^2 \, \mathrm{d}X_m \\ &= \sum_m \int |(D_z\psi_\alpha)_m|^2 \prod_{i<j}^m (1 - \eta(x_i - x_j)) \, \mathrm{d}X_m. \end{aligned} \tag{3.6.16}$$

The product in the integral can be estimated as follows. It is easy to show that if a_k are numbers between zero and one we have

$$\prod_{k=1}^n (1 - a_k) \geq 1 - \sum_{k=1}^n a_k \tag{3.6.17}$$

for $n \in \mathbb{N}$. Then we use that the ψ_α are normalized and D_z as a unitary operator does not change that. Hence

$$\|fD_z\psi_\alpha\|^2 \geq 1 - \sum_m \sum_{i<j}^m \int |(D_z\psi_\alpha)_m|^2 \eta(x_i - x_j) \, \mathrm{d}X_m. \tag{3.6.18}$$

We can now perform the integration over all but two coordinates of $|(D_z\psi_\alpha)_m|^2$ to write

$$\begin{aligned} &\sum_m \sum_{i<j}^m \int |(D_z\psi_\alpha)_m|^2 \eta(x_i - x_j) \, \mathrm{d}X_m \\ &= \sum_m \sum_{i<j}^m \int \eta(x_i - x_j) \left(\int |(D_z\psi_\alpha)_m|^2 \, \mathrm{d}\hat{X}_{i,j} \right) \mathrm{d}x_i \, \mathrm{d}x_j \\ &= \frac{1}{2} \int \eta(x - y) \rho^{(2)}_{\alpha,z}(x, y) \, \mathrm{d}x \, \mathrm{d}y, \end{aligned} \tag{3.6.19}$$

where $\mathrm{d}\hat{X}_{i,j}$ as before denotes integration over all variables except x_i and x_j and we used the permutation symmetry of ψ_α. In the last step we recognized the two-particle density of the state $D_z\psi_\alpha$

$$\rho^{(2)}_{\alpha,z}(x, y) = \langle a_x^\dagger a_y^\dagger a_y a_x \rangle_{D_z\psi_\alpha}. \tag{3.6.20}$$

Using (3.6.11), this can be evaluated as

$$\begin{aligned}
\rho^{(2)}_{\alpha,z}(x,y) &= \langle D_z^\dagger a_x^\dagger D_z D_z^\dagger a_y^\dagger D_z D_z^\dagger a_y D_z D_z^\dagger a_x D_z \rangle_{\psi_\alpha} \\
&= \langle (a_x^\dagger + \bar{z}/\tilde{\ell})(a_y^\dagger + \bar{z}/\tilde{\ell})(a_y + z/\tilde{\ell})(a_x + z/\tilde{\ell}) \rangle_{\psi_\alpha} \\
&= |z|^4 \tilde{\ell}^{-4} + |z|^2 \tilde{\ell}^{-2} \left(\langle a_x^\dagger a_y \rangle_{\psi_\alpha} + \langle a_x^\dagger a_x \rangle_{\psi_\alpha} + \langle a_y^\dagger a_y \rangle_{\psi_\alpha} + \langle a_y^\dagger a_x \rangle_{\psi_\alpha} \right) + \langle a_x^\dagger a_y^\dagger a_y a_x \rangle_{\psi_\alpha} \\
&= |z|^4 \tilde{\ell}^{-4} + |z|^2 \tilde{\ell}^{-2} \left(\gamma_\alpha(x,y) + \rho_\alpha(x) + \rho_\alpha(y) + \gamma_\alpha(y,x) \right) + \rho^{(2)}_\alpha(x,y). \qquad (3.6.21)
\end{aligned}$$

The one- and two-particle densities of the state ψ_α appearing in the calculation can be estimated explicitly. By inserting the plane wave expansion $a_x = \sum_p a_p \,\mathrm{e}^{ipx}\, \tilde{\ell}^{-1}$, we find for the one-particle density

$$\rho_\alpha(x) = \langle a_x^\dagger a_x \rangle_{\psi_\alpha} = \sum_{p,q} \frac{\mathrm{e}^{ix(p-q)}}{\tilde{\ell}^2} \langle a_p^\dagger a_q \rangle_{\psi_\alpha} = \sum_p \frac{1}{\tilde{\ell}^2} \langle n_p \rangle_{\psi_\alpha} = \frac{N_\alpha}{\tilde{\ell}^2}. \qquad (3.6.22)$$

Since $\gamma_\alpha(x,y) \leq \gamma_\alpha(x,x) = \rho_\alpha(x)$, we also have a bound on the one-particle density matrix. Similarly, the two-particle density is estimated as

$$\begin{aligned}
\rho^{(2)}_\alpha(x,y) = \langle a_x^\dagger a_y^\dagger a_y a_x \rangle_{\psi_\alpha} &= \frac{1}{\tilde{\ell}^4} \sum_{p_1,p_2,p_3,p_4} \mathrm{e}^{ip_1 x}\, \mathrm{e}^{ip_2 y}\, \mathrm{e}^{-ip_3 y}\, \mathrm{e}^{-ip_4 x} \langle a_{p_4}^\dagger a_{p_3}^\dagger a_{p_2} a_{p_1} \rangle_{\psi_\alpha} \\
&= \frac{1}{\tilde{\ell}^4} \sum_p \langle a_p^\dagger a_p^\dagger a_p a_p \rangle_{\psi_\alpha} + \frac{1}{\tilde{\ell}^4} \sum_{p_1 \neq p_2} \langle a_{p_1}^\dagger a_{p_2}^\dagger a_{p_2} a_{p_1} \rangle_{\psi_\alpha} \\
&\quad + \frac{1}{\tilde{\ell}^4} \sum_{p_1 \neq p_2} \mathrm{e}^{ip_1(x-y)}\, \mathrm{e}^{ip_2(y-x)} \langle a_{p_1}^\dagger a_{p_2}^\dagger a_{p_1} a_{p_2} \rangle_{\psi_\alpha} \\
&\leq \frac{1}{\tilde{\ell}^4} \sum_p n_p(n_p - 1) + \frac{2}{\tilde{\ell}^4} \sum_{p_1 \neq p_2} n_{p_1} n_{p_2} \\
&\leq \frac{2}{\tilde{\ell}^4} \sum_{p_1,p_2} n_{p_1} n_{p_2} = 2 \frac{N_\alpha^2}{\tilde{\ell}^4}. \qquad (3.6.23)
\end{aligned}$$

For $\alpha \in \mathcal{A}$, we use the uniform bound $N_\alpha < \mathcal{N}$ and hence

$$\|f D_z \psi_\alpha\|^2 \geq 1 - \frac{1}{2\tilde{\ell}^2} \int \eta \left(|z|^4 + 4|z|^2 \mathcal{N} + 2\mathcal{N}^2 \right) \geq 1 - \frac{\pi R^2}{2\tilde{\ell}^2} \left(|z|^4 + 2|z|^2 \mathcal{N} + 2\mathcal{N}^2 \right). \quad (3.6.24)$$

In the last inequality we estimated $\eta \leq 1$ on the disk of radius R. □

The second lemma is about the set $\mathcal{A}$ that was introduced to be able to give a uniform bound in the norm estimate.

Lemma 15 (Particle number estimate)**.** *We have for any* $0 < k < 1$ *the following estimates*

$$\sum_{\alpha\in\mathcal{A}} \lambda_\alpha \geq 1 - \exp\left[-k\beta|\mu_0|\mathcal{N} + \tau(\beta\mu_0, k)n_G\right] =: \frac{1}{B_2}$$
$$\sum_{\alpha\notin\mathcal{A}} \lambda_\alpha N_\alpha \leq n_G \exp\left[-k\beta|\mu_0|\mathcal{N} + \tau(\beta\mu_0, k)n_G\right]. \tag{3.6.25}$$

Here, τ *is given by*

$$\tau(\beta\mu_0, k) = -\left(\mathrm{e}^{-\beta\mu_0} - 1\right) \ln\left(1 - \frac{\mathrm{e}^{-k\beta\mu_0} - 1}{\mathrm{e}^{-\beta\mu_0} - 1}\right). \tag{3.6.26}$$

Proof. We have

$$\sum_{\alpha\in\mathcal{A}} \lambda_\alpha = 1 - \sum_{\alpha\notin\mathcal{A}} \lambda_\alpha = 1 - \langle \chi_{\mathbb{N}\geq\mathcal{N}} \rangle_{\Gamma_G}. \tag{3.6.27}$$

The characteristic function can be estimated by an exponential function with parameter $\varkappa > 0$ as

$$\langle \chi_{\mathbb{N}\geq\mathcal{N}} \rangle_{\Gamma_G} \leq \langle \mathrm{e}^{\varkappa(\mathbb{N}-\mathcal{N})} \rangle_{\Gamma_G}. \tag{3.6.28}$$

Furthermore, the expectation is immediately obtained as

$$\begin{aligned}\langle \mathrm{e}^{\varkappa(\mathbb{N}-\mathcal{N})} \rangle_{\Gamma_G} &= \mathrm{e}^{-\varkappa\mathcal{N}} \frac{\mathrm{Tr}_{\mathcal{F}}\, \mathrm{e}^{-\beta(\mathbb{H}_0 - \mu_0\mathbb{N}) + \varkappa\mathbb{N}}}{\mathrm{Tr}_{\mathcal{F}}\, \mathrm{e}^{-\beta(\mathbb{H}_0 - \mu_0\mathbb{N})}} \\ &= \exp\left(\beta\tilde{\ell}^2 \left[P_{\tilde{\ell}}(\beta, \mu_0 + \varkappa/\beta) - P_{\tilde{\ell}}(\beta, \mu_0)\right] - \varkappa\mathcal{N}\right).\end{aligned} \tag{3.6.29}$$

Here, $P_{\tilde{\ell}}(\beta, \mu_0)$ is the grand canonical pressure of the Gibbs state in finite volume. It can be explicitly computed as

$$\begin{aligned}P_{\tilde{\ell}}(\beta, \mu_0) &= \frac{1}{\beta\tilde{\ell}^2} \ln Z_0 = \frac{1}{\beta\tilde{\ell}^2} \ln \mathrm{Tr}_{\mathcal{F}}\, \mathrm{e}^{-\beta(\mathbb{H}_0 - \mu_0\mathbb{N})} \\ &= -\frac{1}{\beta\tilde{\ell}^2} \sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2} \ln\left(1 - \mathrm{e}^{-\beta(p^2 - \mu_0)}\right).\end{aligned} \tag{3.6.30}$$

We find for the difference

$$\begin{aligned}P_{\tilde{\ell}}(\beta, \mu_0 + \varkappa/\beta) - P_{\tilde{\ell}}(\beta, \mu_0) &= -\frac{1}{\beta\tilde{\ell}^2} \sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2} \ln\left(\frac{1 - \mathrm{e}^{-\beta(p^2 - \mu_0) + \varkappa}}{1 - \mathrm{e}^{-\beta(p^2 - \mu_0)}}\right) \\ &= -\frac{1}{\beta\tilde{\ell}^2} \sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2} \ln\left(1 - \frac{\mathrm{e}^{\varkappa} - 1}{\mathrm{e}^{\beta(p^2 - \mu_0)} - 1}\right).\end{aligned} \tag{3.6.31}$$

We see that $\varkappa$ has to be in the range $0 < \varkappa < -\beta\mu_0 = \beta|\mu_0|$ in order for the $p = 0$ term not to blow up. Therefore, we parametrize $\varkappa$ as $\varkappa = -k\beta\mu_0$ for $0 < k < 1$. It will be convenient to estimate $-\ln(1-x) \leq \eta x$ where η is chosen such that equality occurs for the biggest x considered. In our case that means

$$\eta = -\left(\frac{\mathrm{e}^{-k\beta\mu_0}-1}{\mathrm{e}^{-\beta\mu_0}-1}\right)^{-1} \ln\left(1 - \frac{\mathrm{e}^{-k\beta\mu_0}-1}{\mathrm{e}^{-\beta\mu_0}-1}\right). \tag{3.6.32}$$

The benefit of doing this estimate is that the sum over p can then be evaluated as the density of the Gibbs state:

$$\begin{aligned} P_{\tilde{\ell}}(\beta, \mu_0(1-k)) - P_{\tilde{\ell}}(\beta, \mu_0) &\leq \frac{1}{\beta\tilde{\ell}^2} \sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2} \eta \frac{\mathrm{e}^{-k\beta\mu_0}-1}{\mathrm{e}^{\beta(p^2-\mu_0)}-1} \\ &= \eta\left(\mathrm{e}^{-k\beta\mu_0}-1\right)\frac{n_G}{\beta\tilde{\ell}^2} = \tau(\beta\mu_0, k)\frac{n_G}{\beta\tilde{\ell}^2}. \end{aligned} \tag{3.6.33}$$

Hence

$$\sum_{\alpha\in\mathcal{A}} \lambda_\alpha \geq 1 - \mathrm{e}^{-k\beta|\mu_0|(\mathcal{N}-\tau(\beta\mu_0,k)n_G)}. \tag{3.6.34}$$

To show the second inequality, one only needs to realize that

$$\mathrm{Tr}_{\mathcal{F}}\left[\mathbb{N}\,\mathrm{e}^{-\beta(\mathbb{H}-\mu_0\mathbb{N})+\varkappa\mathbb{N}}\right] = \frac{\partial}{\partial\varkappa}\mathrm{Tr}_{\mathcal{F}}\left[\mathrm{e}^{-\beta(\mathbb{H}-\mu_0\mathbb{N})+\varkappa\mathbb{N}}\right] \tag{3.6.35}$$

and can then follow the same arguments as above. □

Remark. It should be noted that, according to the definition of n_G in (3.6.13), the quantities on the left-hand side of (3.6.25) reappear on the right-hand side. Using $\sum_{\alpha\in\mathcal{A}}\lambda_\alpha \leq 1$ as well as assuming that the first term in the exponential, $-k\beta|\mu_0|\mathcal{N}$, dominates the second term, $\tau(\beta\mu_0, k)n_G$, we see that this recursion leads to a tower of exponentials with negative exponent.

In the third lemma of this subsection we estimate the expectation value of the Hamiltonian, i.e., the energy $\mathrm{Tr}_{\mathcal{F}}\,\mathbb{H}\Gamma$, where $\mathbb{H}$ is the Fock space Hamiltonian with periodic boundary conditions. We have

$$\begin{aligned} \mathrm{Tr}_{\mathcal{F}}\,\mathbb{H}\Gamma &= \sum_{\alpha\in\mathcal{A}} \frac{\tilde{\lambda}_\alpha}{\|fD_z\psi_\alpha\|^2}\langle fD_z\psi_\alpha|\mathbb{H}|fD_z\psi_\alpha\rangle \\ &= \sum_{\alpha\in\mathcal{A}} \frac{\tilde{\lambda}_\alpha}{\|fD_z\psi_\alpha\|^2}\sum_m \int f_m\overline{(D_z\psi_\alpha)_m}H_m f_m(D_z\psi_\alpha)_m\,\mathrm{d}X_m, \end{aligned} \tag{3.6.36}$$

where we introduced the shorthand $X_m = (x_1, \dots, x_m)$. Here, H_m is the restriction of $\mathbb{H}$ to the sector of particle number m. In evaluating this integral, we find

$$\begin{aligned}
&\int f_m \overline{(D_z\psi_\alpha)_m} H_m f_m (D_z\psi_\alpha)_m \,\mathrm{d}X_m \\
&\quad = \int f_m \overline{(D_z\psi_\alpha)_m} \left(-\sum_{i=1}^m \Delta_i + \sum_{i<j}^m v(d(x_i, x_j)) \right) f_m (D_z\psi_\alpha)_m \,\mathrm{d}X_m \\
&\quad = \int |\nabla f_m (D_z\psi_\alpha)_m|^2 \,\mathrm{d}X_m + \sum_{i<j}^m \int v(d(x_i, x_j)) |f_m (D_z\psi_\alpha)_m|^2 \,\mathrm{d}X_m.
\end{aligned} \tag{3.6.37}$$

We used integration by parts and the fact that the boundary terms vanish due to periodic boundary conditions. The first term can be rewritten as

$$\begin{aligned}
\int |\nabla f_m (D_z\psi_\alpha)_m|^2 \,\mathrm{d}X_m &= \int |(\nabla f_m)(D_z\psi_\alpha)_m + f_m \nabla (D_z\psi_\alpha)_m|^2 \,\mathrm{d}X_m \\
&= \int \left(|\nabla f_m|^2 |(D_z\psi_\alpha)_m|^2 + f_m^2 |\nabla (D_z\psi_\alpha)_m|^2 \right) \mathrm{d}X_m \\
&\qquad + 2\,\mathrm{Re} \int f_m \overline{(D_z\psi_\alpha)_m} \nabla f_m \cdot \nabla (D_z\psi_\alpha)_m \,\mathrm{d}X_m \\
&= \int \left(|\nabla f_m|^2 |(D_z\psi_\alpha)_m|^2 - f_m^2 \overline{(D_z\psi_\alpha)_m} \Delta (D_z\psi_\alpha)_m \right) \mathrm{d}X_m,
\end{aligned} \tag{3.6.38}$$

where we again used integration by parts. The first term on the right-hand side, together with the potential term in (3.6.37), will be used to obtain the correction to the free energy, while the second term will be used to obtain the leading order contribution coming from the free Bose gas. We define

$$\mathcal{E} := \sum_{\alpha \in \mathcal{A}} \frac{\tilde{\lambda}_\alpha}{\|f D_z \psi_\alpha\|^2} \sum_m \int f_m^2 \overline{(D_z\psi_\alpha)_m} (-\Delta) (D_z\psi_\alpha)_m \,\mathrm{d}X_m. \tag{3.6.39}$$

Observe that the free Hamiltonian $\mathbb{H}_0$ does not "see" the difference between a state with or without added quasi-condensate (since this carries no kinetic energy). This means that if E_α is the eigenvalue of ψ_α, then we have

$$\mathbb{H}_0 D_z \psi_\alpha = E_\alpha D_z \psi_\alpha. \tag{3.6.40}$$

Hence

$$\mathcal{E} = \sum_{\alpha \in \mathcal{A}} \frac{\tilde{\lambda}_\alpha}{\|f D_z \psi_\alpha\|^2} \sum_m \int f_m^2 \overline{(D_z\psi_\alpha)_m} E_\alpha (D_z\psi_\alpha)_m \,\mathrm{d}X_m = \frac{1}{\sum_{\alpha' \in \mathcal{A}} \lambda_{\alpha'}} \sum_{\alpha \in \mathcal{A}} \lambda_\alpha E_\alpha. \tag{3.6.41}$$

Now we evaluate the gradient term on the right-hand side of (3.6.38). We have

$$\nabla_{x_k} f_m = \nabla_{x_k} \prod_{i<j}^{m} g(x_i - x_j) = \sum_{l, l \neq k} \frac{f_m}{g(x_l - x_k)} \nabla_{x_k} g(x_l - x_k), \tag{3.6.42}$$

where we used that g is even in the last equality. Note that the sum in the last line of (3.6.42) is not a double sum. Thus, the square of the gradient of f_m is given by

$$|\nabla f_m|^2 = \sum_k \sum_{l, l' \neq k} (\nabla_{x_k} g)(x_l - x_k) \cdot (\nabla_{x_k} g)(x_{l'} - x_k) \frac{f_m^2}{g(x_l - x_k) g(x_{l'} - x_k)}. \tag{3.6.43}$$

We split this sum into a diagonal and an off-diagonal part:

$$\begin{aligned} |\nabla f_m|^2 = {} & 2 \sum_{l<k} \left((\nabla_{x_k} g)(x_l - x_k) \frac{f_m}{g(x_l - x_k)} \right)^2 \\ & + \sum_k \sum_{\substack{l, l' \neq k \\ l \neq l'}} (\nabla_{x_k} g)(x_l - x_k) \cdot (\nabla_{x_k} g)(x_{l'} - x_k) \frac{f_m^2}{g(x_l - x_k) g(x_{l'} - x_k)}. \end{aligned} \tag{3.6.44}$$

The diagonal part contains the squared gradient of g and that is exactly what we need to extract the interaction term. Note that we changed the condition on the first sum to $l < k$ and obtained a factor of two. We define further

$$\begin{aligned} \mathcal{I} := {} & \sum_{\alpha \in \mathcal{A}} \frac{2\tilde{\lambda}_\alpha}{\|f D_z \psi_\alpha\|^2} \sum_m \sum_{i<j} \\ & \times \int \left(|\nabla_{x_j} g(x_i - x_j)|^2 + v(x_i - x_j) g(x_i - x_j)^2 \right) \frac{f_m^2}{g(x_i - x_j)^2} |(D_z \psi_\alpha)_m|^2 \, \mathrm{d}X_m, \\ \mathcal{R} := {} & \sum_{\alpha \in \mathcal{A}} \frac{\tilde{\lambda}_\alpha}{\|f D_z \psi_\alpha\|^2} \sum_m \sum_k \sum_{\substack{l, l' \neq k \\ l \neq l'}} \\ & \times \int (\nabla_{x_k} g)(x_l - x_k) \cdot (\nabla_{x_k} g)(x_{l'} - x_k) \frac{f_m^2}{g(x_l - x_k) g(x_{l'} - x_k)} |(D_z \psi_\alpha)_m|^2 \, \mathrm{d}X_m. \end{aligned} \tag{3.6.45}$$

Lemma 16 (Energy estimate)**.** *With the definitions above, we have*

$$\mathrm{Tr}_{\mathcal{F}} \, \mathbb{H}\Gamma = \mathcal{E} + \mathcal{I} + \mathcal{R}. \tag{3.6.46}$$

We define $|z|^2 = n_0$ and give bounds for each term separately. For the first one, we have

$$\mathcal{E} \leq B_2 \operatorname{Tr}_{\mathcal{F}} \mathbb{H}_0 \Gamma_G, \tag{3.6.47}$$

where $\mathbb{H}_0$ is the non-interacting Hamiltonian on Fock space with periodic boundary conditions and Γ_G is the grand canonical Gibbs state introduced above. For the second term we have

$$\mathcal{I} \leq \frac{2\pi B_1 B_2}{\ln(R/a)\tilde{\ell}^2}\left(n_0^2 + 4n_0 n_G + 2n_G^2\right)\left(1 + \frac{C}{\ln(R/a)}\right) \tag{3.6.48}$$

and for the third one

$$\mathcal{R} \leq 34 B_1 B_2 \frac{n^3}{\tilde{\ell}^4}\frac{R^2}{\ln^2(R/a)}. \tag{3.6.49}$$

The multiplicative errors B_1 and B_2 are given in Lemma 14 and 15.

Proof. For the first inequality we continue the calculation from (3.6.41) and simply add back the missing terms to the sum to obtain the expectation of the free Hamiltonian in the Gibbs state as well as use Lemma 15

$$\mathcal{E} = \frac{1}{\sum_{\alpha' \in \mathcal{A}} \lambda_{\alpha'}} \sum_{\alpha \in \mathcal{A}} \lambda_\alpha E_\alpha \leq B_2 \sum_\alpha \lambda_\alpha E_\alpha = B_2 \operatorname{Tr}_{\mathcal{F}} \mathbb{H}_0 \Gamma_G. \tag{3.6.50}$$

For the second inequality, we introduce the function

$$\xi(x) = |\nabla g(d(x,0))|^2 + \frac{1}{2} v(d(x,0)) g(d(x,0))^2. \tag{3.6.51}$$

Similarly as in the proof of the norm estimate, we integrate out all but two variables to find the two-particle density. To do so, we estimate the remaining factors of g in the integral by one:

$$\begin{aligned}
\mathcal{I} &= \sum_{\alpha \in \mathcal{A}} \frac{2\tilde{\lambda}_\alpha}{\|f D_z \psi_\alpha\|^2} \sum_m \sum_{i<j} \int \left(\xi(x_i - x_j) \int \frac{f_m^2}{g(x_i - x_j)^2} |(D_z \psi_\alpha)_m|^2 \, \mathrm{d}\hat{X}_{i,j} \right) \mathrm{d}x_i x_j \\
&\leq \sum_{\alpha \in \mathcal{A}} \frac{2\tilde{\lambda}_\alpha}{\|f D_z \psi_\alpha\|^2} \sum_m \sum_{i<j} \int \left(\xi(x_i - x_j) \int |(D_z \psi_\alpha)_m|^2 \, \mathrm{d}\hat{X}_{i,j} \right) \mathrm{d}x_i x_j \\
&\leq B_1 B_2 \sum_\alpha \lambda_\alpha \int \xi(x-y) \rho^{(2)}_{\alpha,z}(x,y) \, \mathrm{d}x \, \mathrm{d}y \\
&= B_1 B_2 \int \xi(x-y) \rho^{(2)}_z(x,y) \, \mathrm{d}x \, \mathrm{d}y.
\end{aligned} \tag{3.6.52}$$

In the last inequality, we have used Lemma 14 and 15 as well as added back the missing terms to the sum in order to obtain the full two-particle density of the Gibbs state with manually added condensate $\rho_z^{(2)}(x,y)$ in the last equality. We have

$$\rho_z^{(2)}(x,y) = \langle a_x^\dagger a_y^\dagger a_y a_x \rangle_{D_z \Gamma_G D_z^\dagger} . \tag{3.6.53}$$

Since Γ_G is quasi-free, we can apply Wick's theorem. It states that for any quasi-free state the expectation value of products of creation/annihilation operators is zero for an odd number of factors and for an even number of factors it is given by a sum of terms that contain only expectation values of two operators,

$$\langle c_1 \cdots c_{2n} \rangle_{\Gamma_G} = \sum_\pi \langle c_{\pi(1)} c_{\pi(2)} \rangle_{\Gamma_G} \cdots \langle c_{\pi(2n-1)} c_{\pi(2n)} \rangle_{\Gamma_G} , \tag{3.6.54}$$

where the sum runs over all ordered permutations π of the set $\{1, \dots, 2n\}$ and the c_j are either creation or annihilation operators. Ordered permutations are those permutations π such that

$$\pi(2j-1) < \pi(2j+1),\ j = 1, \dots, n-1 \quad \text{and} \quad \pi(2j-1) < \pi(2j),\ j = 1, \dots, n. \tag{3.6.55}$$

Using Wick's theorem and (3.6.11), we calculate

$$\begin{aligned} \langle a_x^\dagger a_y^\dagger a_y a_x \rangle_{D_z \Gamma_G D_z^\dagger} &= \langle D_z^\dagger a_x^\dagger a_y^\dagger a_y a_x D_z \rangle_{\Gamma_G} \\ &= \langle (a_x^\dagger + \bar{z}/\tilde{\ell})(a_y^\dagger + \bar{z}/\tilde{\ell})(a_y + z/\tilde{\ell})(a_x + z/\tilde{\ell}) \rangle_{\Gamma_G} \\ &= |z|^4 \tilde{\ell}^{-4} + |z|^2 \tilde{\ell}^{-2} (\rho(x) + \rho(y) + \gamma(x,y) + \gamma(y,x)) + |\gamma(x,y)|^2 + \rho(x)\rho(y). \end{aligned} \tag{3.6.56}$$

Similarly as before (compare the estimates following (3.6.20)), we estimate this by

$$\rho_z^{(2)}(x,y) \le \frac{1}{\tilde{\ell}^4} \left(|z|^4 + 4|z|^2 n_G + 2n_G^2 \right), \tag{3.6.57}$$

where n_G is the number of particles in the Gibbs state, see (3.6.13). Now we use (3.3.10) and write

$$\begin{aligned} \int_{|x| \le \tilde{\ell}} \xi &= \int_{B_R} \left(|\nabla g_0|^2 + \frac{1}{2} v |g_0|^2 \right) + \frac{1}{2} \int_{R \le |x| \le \tilde{\ell}} v(|x|) \, \mathrm{d}x \\ &= \frac{2\pi}{\ln(R/a_R)} + \frac{1}{2} \int_{R \le |x| \le \tilde{\ell}} v(|x|) \, \mathrm{d}x. \end{aligned}$$

The first term on the right-hand side can be estimated using (3.3.11), while the second term can be bounded using (1.2.15) as

$$\frac{1}{2}\int_{R\le|x|\le\tilde{\ell}} v(|x|)\,\mathrm{d}x \le \frac{1}{2\ln^2(R/a)}\int_{|x|\ge R} v(|x|)\ln^2(|x|/a)\,\mathrm{d}x \le \frac{2\pi C}{\ln^2(R/a)}, \tag{3.6.58}$$

where $C>0$ is a constant. Then we continue the estimate from (3.6.52) as

$$\begin{aligned} \mathcal{I} &\le B_1B_2\tilde{\ell}^{-2}\left(|z|^4+4|z|^2n_G+2n_G^2\right)\int_{|x|\le\tilde{\ell}}\xi \\ &\le B_1B_2\tilde{\ell}^{-2}\left(|z|^4+4|z|^2n_G+2n_G^2\right)\left(\frac{2\pi}{\ln(R/a)}+\frac{2\pi C}{\ln^2(R/a)}\right). \end{aligned} \tag{3.6.59}$$

Inserting now $|z|^2=n_0$, this becomes

$$\mathcal{I} \le \frac{2\pi B_1B_2}{\ln(R/a)\tilde{\ell}^2}\left(n_0^2+4n_0n_G+2n_G^2\right)\left(1+\frac{C}{\ln(R/a)}\right). \tag{3.6.60}$$

Lastly, we estimate the three-particle term $\mathcal{R}$. The remaining factors of g are bounded by one and we insert the definition of the three-particle density:

$$\begin{aligned} \mathcal{R} &= \sum_{\alpha\in\mathcal{A}}\frac{\tilde{\lambda}_\alpha}{\|fD_z\psi_\alpha\|^2}\sum_k\sum_{\substack{l,l'\neq k\\ l\neq l'}} \\ &\quad\times\int(\nabla_{x_k}g)(x_l-x_k)\cdot(\nabla_{x_k}g)(x_{l'}-x_k)\frac{f_m^2}{g(x_l-x_k)g(x_{l'}-x_k)}|(D_z\psi_\alpha)_{n_\alpha}|^2\,\mathrm{d}X_m \\ &\le B_1B_2\int(\nabla_xg)(x-z)\cdot(\nabla_yg)(y-z)\rho_z^{(3)}(x,y,z)\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z. \end{aligned} \tag{3.6.61}$$

The three-particle density is estimated as[2]

$$\begin{aligned} \rho_z^{(3)}(x,y,z) &= \langle a_x^\dagger a_y^\dagger a_z^\dagger a_za_ya_x\rangle_{D_z\Gamma_GD_z^\dagger} \\ &= \langle(a_x^\dagger+\bar{z}/\tilde{\ell})(a_y^\dagger+\bar{z}/\tilde{\ell})(a_z^\dagger+\bar{z}/\tilde{\ell})(a_z+z/\tilde{\ell})(a_y+z/\tilde{\ell})(a_x+z/\tilde{\ell})\rangle_{\Gamma_G} \\ &= \langle a_x^\dagger a_y^\dagger a_z^\dagger a_za_ya_x\rangle_{\Gamma_G}+\frac{|z|^4}{\tilde{\ell}^4}\left(\langle a_x^\dagger a_x\rangle_{\Gamma_G}+8\text{ other terms}\right)+\frac{|z|^6}{\tilde{\ell}^6} \\ &\quad+\frac{|z|^2}{\tilde{\ell}^2}\left(\langle a_x^\dagger a_y^\dagger a_ya_x\rangle_{\Gamma_G}+8\text{ other terms}\right). \end{aligned} \tag{3.6.62}$$

[2]Beware of the slight abuse of notation: the index z refers to the coherent state parameter, while the arguments of $\rho_z^{(3)}$ are the coordinates (x,y,z) in $\Lambda_{\tilde{\ell}}$

The first term is the three-particle density of the Gibbs state and is evaluated using again Wick's theorem, the resulting bound is $\rho^{(3)} \leq 6n_G^3/\tilde{\ell}^6$. If we insert now $|z|^2 = n_0$ and estimate all occurrences of n_0 and n_G by n, we find that

$$\rho_z^{(3)}(x, y, z) \leq 34\frac{n^3}{\tilde{\ell}^6}. \tag{3.6.63}$$

Thus, for a simple bound, we can apply part 3 of Lemma 10 (and then (3.3.11)) and estimate $\mathcal{R}$ further as

$$\mathcal{R} \leq 34B_1B_2\tilde{\ell}^2\frac{n^3}{\tilde{\ell}^6}\frac{R^2}{\ln^2(R/a)}. \tag{3.6.64}$$

□

Finally, we need to estimate the entropy of the trial state Γ in order to obtain a bound on the free energy. We relate the entropy of Γ to the entropy of the Gibbs state Γ_G such that adding to it the energy $\mathrm{Tr}_{\mathcal{F}}\, \mathbb{H}_0\Gamma_G$ we obtain the free energy of Γ_G.

Lemma 17 (Entropy estimate)**.** *We have*

$$S(\Gamma) - B_2S(\Gamma_G) \geq -B_2 \ln B_2 - \ln B_1, \tag{3.6.65}$$

where B_1 and B_2 are defined in Lemma 14 and 15.

Proof. The proof relies on [69, proof of Lemma 2] and for the reader's convenience we repeat it here. For $\{P_\alpha\}$ a family of rank one projections (not necessarily mutually orthogonal) set $\hat{\Gamma} = \sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha P_\alpha$ and $\tilde{\Gamma}$ a density matrix with eigenvalues $\tilde{\lambda}_\alpha$, $\alpha \in \mathcal{A}$. Then we have by the concavity of the logarithm that

$$\begin{aligned} S(\hat{\Gamma}) - S(\tilde{\Gamma}) &= -\sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha \,\mathrm{Tr}_{\mathcal{F}}\, P_\alpha \ln\left(\tilde{\lambda}_\alpha^{-1}\hat{\Gamma}\right) \\ &\geq -\sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha \ln \mathrm{Tr}_{\mathcal{F}}\, P_\alpha\tilde{\lambda}_\alpha^{-1}\hat{\Gamma} \\ &\geq -\ln \mathrm{Tr}_{\mathcal{F}}\left(\sum_{\alpha\in\mathcal{A}} P_\alpha\hat{\Gamma}\right) \geq -\ln\left\|\sum_{\alpha\in\mathcal{A}} P_\alpha\right\|. \end{aligned} \tag{3.6.66}$$

Then we calculate

$$\begin{aligned} S(\tilde{\Gamma}) &= -\sum_{\alpha\in\mathcal{A}} \tilde{\lambda}_\alpha \ln \tilde{\lambda}_\alpha \\ &= -\sum_{\alpha\in\mathcal{A}} \frac{\lambda_\alpha}{\sum_{\alpha'\in\mathcal{A}} \lambda_{\alpha'}} \ln\left(\frac{\lambda_\alpha}{\sum_{\alpha'\in\mathcal{A}} \lambda_{\alpha'}}\right) \\ &\geq -B_2 \sum_{\alpha\in\mathcal{A}} \lambda_\alpha \left(\ln \lambda_\alpha - \ln \sum_{\alpha'\in\mathcal{A}} \lambda_{\alpha'}\right) \\ &\geq -B_2 \sum_{\alpha} \lambda_\alpha \ln \lambda_\alpha - B_2 \ln B_2 \\ &= B_2 S(\Gamma_G) - B_2 \ln B_2. \end{aligned} \tag{3.6.67}$$

In the last inequality we have recognized $S(\Gamma_G)$, the entropy of the full Gibbs state with eigenvalues λ_α. We used Lemma 15 to estimate the sum $\sum_{\alpha'\in\mathcal{A}} \lambda_{\alpha'}$.

Analogously as in [69, discussion after Lemma 2], we then find for our trial state (inserting $\hat{\Gamma} = \Gamma$)

$$S(\Gamma) - B_2 S(\Gamma_G) \geq -B_2 \ln B_2 - \ln \left\| \sum_{\alpha\in\mathcal{A}} \frac{|f D_z \psi_\alpha\rangle\langle f D_z \psi_\alpha|}{\|f D_z \psi_\alpha\|^2} \right\|. \tag{3.6.68}$$

Define $\chi = \max_{\alpha\in\mathcal{A}} \|f D_z \psi_\alpha\|^{-2}$. Using the fact that $f_k \leq 1$ and the orthonormality of $D_z \psi_\alpha$ (which follows from the orthonormality of ψ_α and the unitarity of D_z), we have

$$\sum_{\alpha\in\mathcal{A}} \frac{|f D_z \psi_\alpha\rangle\langle f D_z \psi_\alpha|}{\|f D_z \psi_\alpha\|^2} \leq \chi \sum_{\alpha\in\mathcal{A}} |f D_z \psi_\alpha\rangle\langle f D_z \psi_\alpha| \leq \chi. \tag{3.6.69}$$

Since $\chi \leq B_1$ (from Lemma 14), we obtain

$$S(\Gamma) - B_2 S(\Gamma_G) \geq -B_2 \ln B_2 - \ln B_1. \tag{3.6.70}$$

□

3.7 Final upper bound

Now that we have an estimate for every term appearing in the free energy functional, we are ready to state the upper bound on the free energy. Using Lemmas 14–17, we have the following upper bound on the free energy in finite volume of the trial state Γ:

$$\begin{aligned}\mathcal{F}^{\beta,\tilde{\ell}}(\Gamma) \leq B_2\Bigg(\frac{1}{\beta}\sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2}\ln\Big(1-\mathrm{e}^{-\beta(p^2-\mu_0)}\Big)+\mu_0(\rho-\rho_0)\tilde{\ell}^2\Bigg)\\ + B_1B_2\frac{4\pi\tilde{\ell}^2\rho^2}{\ln(R/a)}\left(1-\frac{\rho_0^2}{2\rho^2}\right)\\ + 34B_1B_2\frac{\tilde{\ell}^2\rho^3R^2}{\ln^2(R/a)}+\frac{1}{\beta}B_2\ln B_2+\frac{1}{\beta}\ln B_1.\end{aligned} \tag{3.7.1}$$

We have used the fact that

$$\mathrm{Tr}_{\mathcal{F}}\,\mathbb{H}_0\Gamma_G-\frac{1}{\beta}S(\Gamma_G)=\frac{1}{\beta}\sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2}\ln\Big(1-\mathrm{e}^{-\beta(p^2-\mu_0)}\Big)+\mu_0 n_G. \tag{3.7.2}$$

When replacing the discrete version of the free energy by its continuum version, we obtain another error term. This finite size effect can be estimated using Lemma 9, with the result

$$\begin{aligned}\frac{1}{\tilde{\ell}^2}\Bigg(\frac{1}{\beta}\sum_{p\in(2\pi/\tilde{\ell})\mathbb{Z}^2}\ln(1-\mathrm{e}^{-\beta(p^2-\mu_0)})+\mu_0(\rho-\rho_0)\tilde{\ell}^2\Bigg)-f_0(\beta,\rho-\rho_0)\\ \leq -\frac{1}{\beta\tilde{\ell}\pi}\int_{\mathbb{R}^2}\frac{1}{|p|}\ln\Big(1-\mathrm{e}^{-\beta(p^2-\mu_0)}\Big)\,\mathrm{d}p=\frac{\text{const.}}{\beta^{3/2}\tilde{\ell}}\end{aligned} \tag{3.7.3}$$

for some positive constant.

We still have to estimate the term involving the two-particle density appearing on the right-hand side of (3.5.7). Now that we have chosen the trial state (in (3.6.1)) and have estimates for the two-particle density (from (3.6.57)), we apply Lemmas 14 and 15 to obtain

$$\begin{aligned}\frac{1}{2\ell^2}\sum_{\alpha\in\mathcal{A}}\frac{\tilde{\lambda}_\alpha}{\|fD_z\psi_\alpha\|}\int_{\mathcal{B}^b_{\tilde{\ell}}}v(d(x,y))\rho^{(2)}_{fD_z\psi_\alpha}(x^{\mathrm{R}},y^{\mathrm{R}})h(x)h(y)\,\mathrm{d}x\,\mathrm{d}y\\ \leq \frac{B_1B_2}{2\ell^2}\sum_\alpha\lambda_\alpha\int_{\mathcal{B}^b_{\tilde{\ell}}}v(d(x,y))g^2(d(x,y))\rho^{(2)}_{\alpha,z}(x^{\mathrm{R}},y^{\mathrm{R}})\,\mathrm{d}x\,\mathrm{d}y\\ \leq \frac{bB_1B_2}{2\ell^2\tilde{\ell}^3}\Big(n_0^2+4n_0n_G+2n_G^2\Big)\left(\frac{2\pi}{\ln(R/a)}+\frac{2\pi C}{\ln^2(R/a)}\right).\end{aligned} \tag{3.7.4}$$

Therefore, we find for the upper bound on the free energy from (3.5.7) using the estimates from (3.7.1), (3.7.3) and (3.7.4)

$$\begin{aligned} f(\beta,\rho) \leq B_2 f_0(\beta,\rho_G) &+ \frac{\text{const.}B_2}{\beta^{3/2}\ell} + \frac{2\pi B_1 B_2}{\ln(R/a)\ell^2\tilde{\ell}^2}\left(n_0^2 + 4n_0 n_G + 2n_G^2\right)\left(1 + \frac{C}{\ln(R/a)}\right) \\ &+ \frac{34 B_1 B_2 n^3 R^2}{\ell^2\tilde{\ell}^4\ln^2(R/a)} + \frac{1}{\beta\ell^2}(B_2\ln B_2 + \ln B_1) + \frac{4\rho^2}{b^2\rho} + \frac{C\rho^2}{\ln^2(R/a)} \\ &+ \frac{b\pi B_1 B_2}{\ell^2\tilde{\ell}^3\ln(R/a)}\left(n_0^2 + 4n_0 n_G + 2n_G^2\right)\left(1 + \frac{C}{\ln(R/a)}\right). \end{aligned} \tag{3.7.5}$$

Here, we have used $\tilde{\ell}/\ell \leq 1$ to simplify the bound. To simplify it even further, we perform the following replacements. We write $B_1 = 1 + b_1$ and $B_2 = 1 + b_2$ as well as expand the terms with $\tilde{\ell} = \ell - 2b$. We will choose R in the next section on a scale relative to $\rho^{-1/2}$ such that

$$\ln(R/a) = \frac{1}{2}\left(|\ln a^2\rho| - |\ln R^2\rho|\right). \tag{3.7.6}$$

Furthermore, we insert the value for $n_G = (n - n_0)\sum_{\alpha\in\mathcal{A}}\lambda_\alpha + \sum_{\alpha\notin\mathcal{A}}\lambda_\alpha N_\alpha$ from (3.6.13). We use $\sum_{\alpha\in\mathcal{A}}\lambda_\alpha \leq 1$ and the second inequality in Lemma 15. After having done these replacements, we find

$$\begin{aligned} f(\beta,\rho) \leq f_0(\beta,\rho-\rho_0) &+ \frac{4\pi}{|\ln a^2\rho|}\left(2\rho^2 - \rho_0^2\right) \\ &+ b_2\ell^2\rho f_0(\beta,\rho-\rho_0) + \frac{\text{const.}}{\beta^{3/2}\ell} + \frac{\rho^2}{|\ln a^2\rho|}(b_1 + b_2) + \frac{4\pi|\ln R^2\rho|}{|\ln a^2\rho|^2}\left(2\rho^2 - \rho_0^2\right) \\ &+ \frac{1}{\beta\ell^2}(b_1 + b_2) + \frac{4\rho^2}{b^2\rho} + \frac{\rho^2 b}{|\ln a^2\rho|\ell} + \text{higher order terms}. \end{aligned} \tag{3.7.7}$$

The first two terms on the right-hand side are the free energy of the ideal gas and the desired interaction energy, while the remaining terms are error terms. Here, we have suppressed all higher order terms that are not relevant for choosing the optimal error rate. We optimize over all error terms in the next section.

3.8 Choice of parameters

Throughout this section, we use the short hand notation

$$\sigma := |\ln a^2\rho|. \tag{3.8.1}$$

For the optimal choice of the error terms, only the scaling behavior of the parameters is important and we therefore ignore constant factors for these terms. The main terms we have to consider for the minimization are

$$\frac{\rho^2}{\sigma}\left(b_1 + b_2 + \frac{|\ln R^2\rho|}{\sigma} + \frac{\sigma}{\beta\rho\ell^2\rho}(b_1 + b_2) + \frac{b}{\ell} + \frac{\sigma}{b^2\rho} + \frac{\sigma}{(\beta\rho)^{3/2}\ell\rho^{1/2}}\right). \tag{3.8.2}$$

The parameter b is immediately optimized since there are only two terms among the main terms containing b. The result is

$$b^2\rho = \sigma^{2/3}(\ell^2\rho)^{1/3}. \tag{3.8.3}$$

The resulting error term containing b is then proportional to $\rho^2\sigma^{-2/3}(\ell^2\rho)^{-1/3}$. We note that $\tau(\beta\mu_0, k)$ defined in (3.6.26) can be expanded around zero (in both arguments) with the result $\tau(\beta\mu_0, k) \approx -\beta\mu_0 k$, which implies $b_2 \approx \mathrm{e}^{-k\beta|\mu_0|(\mathcal{N}-n)}$. To guarantee exponential decay, we may choose $\mathcal{N}$ as a multiple of $n = \ell^2\rho$. We use that b_2 can be bounded as $b_2 \leq \mathrm{e}^{-\tilde{k}\beta|\mu_0|\rho\ell^2}$ for a constant $\tilde{k} > 0$ and $b_1 \sim (R/\ell)^2(\ell^2\rho)^2$ to see that b_2 is irrelevant for choosing ℓ (as long as $\ell^2\rho \gg \sigma$ in the final choice). Therefore we have only two terms that determine how to optimally choose ℓ, which leads to the equation

$$\frac{\rho^2}{\sigma}\frac{\sigma}{(\ell^2\rho)^{1/2}} = \frac{\rho^2}{\sigma}R^2\rho\ell^2\rho. \tag{3.8.4}$$

This is equivalent to

$$\ell^2\rho = \left(\frac{\sigma}{R^2\rho}\right)^{2/3} \tag{3.8.5}$$

and the resulting error term is proportional to $\rho^2\sigma^{-1}(R^2\rho\sigma^2)^{1/3}$. Finally, we are able to choose R since there are only the two terms $\rho^2\sigma^{-1}(R^2\rho\sigma^2)^{1/3}$ and $\rho^2\sigma^{-2}|\ln R^2\rho|$ to consider. This leads to

$$(R^2\rho\sigma^2)^{1/3} = \frac{|\ln R^2\rho|}{\sigma}, \tag{3.8.6}$$

from which we read off that $R^2\rho$ has to be chosen on a power law scale of σ such that $|\ln R^2\rho| \simeq \ln\sigma$ to leading order. We therefore choose

$$R^2\rho = \frac{\ln^3\sigma}{\sigma^5}. \tag{3.8.7}$$

Then the main relative error term is proportional to $\ln\sigma/\sigma$.

As discussed in Remark 5 in Section 1.2, we now insert for ρ_0 the density

$$\rho_{\mathrm{s}} = \rho\left[1 - \frac{\beta_{\mathrm{c}}}{\beta}\right]_+. \tag{3.8.8}$$

Furthermore, we use $f_0(\beta, \rho - \rho_s) \leq f_0(\beta, \rho)$ and continue the estimate from (3.7.7) as

$$f(\beta, \rho) \leq f_0(\beta, \rho) + \frac{4\pi\rho^2}{\sigma}\left(2 - \left[1 - \frac{\beta_c}{\beta}\right]_+^2\right) + \frac{C\rho^2}{\sigma}\frac{\ln\sigma}{\sigma}. \tag{3.8.9}$$

This concludes the proof of Theorem 3.

We remark that the proof is uniform in the potential in a certain sense. When doing estimates over the tail of the potential, one finds a relative error term (relative to the scale of the interaction ρ^2/σ)

$$\frac{1}{\sigma}\int_{|x|>a} v(|x|)\ln^2(|x|/a)\,\mathrm{d}x, \tag{3.8.10}$$

which can be bounded from above by C/σ using (1.2.15), with a constant C that depends on the potential. We tracked these terms throughout the proof and present them in the estimate in (3.7.5). It turns out that these terms are not relevant for choosing the optimal error rate since they are on a much smaller scale.

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Bibliography

[1] M. Abramowitz and I. A. Stegun, eds. *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables*. New York: Dover Publications, Inc., 1965.

[2] J. O. Andersen. “Ground state pressure and energy density of an interacting homogeneous Bose gas in two dimensions”. *Eur. Phys. J. B* **28** (2002), 389.

[3] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wieman, and E. A. Cornell. “Observation of Bose–Einstein condensation in a dilute atomic vapor”. *Science* **269** (1995), 198–201.

[4] F. A. Berezin. “Covariant and contravariant symbols of operators”. *Izv. Akad. Nauk. Ser. Mat.* **36** (1972), 1134–1167. English translation: *USSR Izv.* **6** (1973), 1117–1151.

[5] F. A. Berezin. “General concept of quantization”. *Comm. Math. Phys.* **40** (1975), 153–174.

[6] V. L. Berezinskii. “Destruction of long-range order in one-dimensional and two-dimensional systems having a continuous symmetry group I. Classical systems.” *Sov. Phys. JETP* **32** (1971), 493.

[7] V. L. Berezinskii. “Destruction of long-range order in one-dimensional and two-dimensional systems possessing a continuous symmetry group. II. Quantum systems.” *Sov. Phys. JETP* **34** (1972), 610.

[8] C. Boccato, C. Brennecke, S. Cenatiempo, and B. Schlein. “The excitation spectrum of Bose gases interacting through singular potentials” (2017). arXiv: `1704.04819 [math-ph]`.

[9] C. Boccato, C. Brennecke, S. Cenatiempo, and B. Schlein. “Complete Bose–Einstein condensation in the Gross–Pitaevskii regime”. *Comm. Math. Phys.* **359** (2018), 975–1026.

[10] C. Boccato, C. Brennecke, S. Cenatiempo, and B. Schlein. “Bogoliubov theory in the Gross–Pitaevskii limit”. *Acta Math.* (2019), 219–335.

[11] N. N. Bogoliubov. “On the theory of superfluidity”. *J. Phys. (USSR)* **11** (1947), 23.

[12] S. N. Bose. “Plancks Gesetz und Lichtquantenhypothese”. *Z. Phys.* **26** (1924), 178–181.

[13] B. Brietzke, S. Fournais, and J. P. Solovej. “A simple 2nd order lower bound to the energy of dilute Bose gases” (2019). arXiv: 1901.00539 [math-ph].

[14] B. Brietzke and J. P. Solovej. “The second-order correction to the ground state energy of the dilute Bose gas”. *Ann. Henri Poincaré* **21** (2020), 571–626.

[15] Y. Castin. “Bose–Einstein condensates in atomic gases: simple theoretical results”. *Coherent atomic matter waves. Lecture notes of Les Houches summer school*. Ed. by R. Kaiser, C. Westbrook, and F. David. EDP Sciences and Springer-Verlag, 2001, 1–136.

[16] Y. Castin and C. Mora. “Ground state energy of the two-dimensional weakly interacting Bose gas: first correction beyond Bogoliubov theory”. *Phys. Rev. Lett.* **102** (2009), 180404.

[17] F. Dalfovo, S. Giorgini, L. P. Pitaevskii, and S. Stringari. “Theory of Bose–Einstein condensation in trapped gases”. *Rev. Mod. Phys.* **71** (1999), 463–512.

[18] K. B. Davis, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle. “Bose–Einstein condensation in a gas of sodium atoms”. *Phys. Rev. Lett.* **75** (1995), 3969–3973.

[19] J. Dereziński and M. Napiórkowski. “Excitation spectrum of interacting bosons in the mean-field infinite-volume limit”. *Ann. Henri Poincaré* **15** (2014), 2409–2439.

[20] A. Deuchert, S. Mayer, and R. Seiringer. “The free energy of the two-dimensional dilute Bose gas. I. Lower bound” (2019). arXiv: 1910.03372 [math-ph].

[21] A. Deuchert and R. Seiringer. “Gross–Pitaevskii limit of a homogeneous Bose gas at positive temperature” (2019). arXiv: 1901.11363 [math-ph].

[22] A. Deuchert, R. Seiringer, and J. Yngvason. “Bose–Einstein condensation in a dilute, trapped gas at positive temperature”. *Comm. Math. Phys.* **368** (2019), 723–776.

[23] F. J. Dyson. “Ground-state energy of a hard-sphere gas”. *Phys. Rev.* **106** (1957), 20–26.

[24] A. Einstein. “Quantentheorie des einatomigen idealen Gases”. *Sitzungsber. Preuss. Akad. Wiss.* (1924), 261–267; A. Einstein. “Quantentheorie des einatomigen idealen Gases. Zweite Abhandlung”. *Sitzungsber. Preuss. Akad. Wiss.* (1925), 3–14.

[25] L. Erdős, B. Schlein, and H.-T. Yau. “Ground-state energy of a low-density Bose gas: a second-order upper bound”. *Phys. Rev. A* **78** (2008), 053627.

[26] D. S. Fisher and P. C. Hohenberg. "Dilute Bose gas in two dimensions". *Phys. Rev. B* **37** (1988), 4936–4943.

[27] S. Fournais, M. Napiórkowski, R. Reuvers, and J. P. Solovej. "Ground state energy of a dilute two-dimensional Bose gas from the Bogoliubov free energy functional". *J. Math. Phys.* **60** (2019), 071903.

[28] S. Fournais and J. P. Solovej. "The energy of dilute Bose gases" (2019). arXiv: `1904.06164 [math-ph]`.

[29] A. Giuliani and R. Seiringer. "The ground state energy of the weakly interacting Bose gas at high density". *J. Stat. Phys.* **135** (2009), 915.

[30] P. Grech and R. Seiringer. "The excitation spectrum for weakly interacting bosons in a trap". *Comm. Math. Phys.* **322** (2013), 559–591.

[31] C. Hainzl and R. Seiringer. "General decomposition of radial functions on $\mathbb{R}^n$ and applications to N-body quantum systems". *Lett. Math. Phys.* **61** (2002), 75–84.

[32] P. C. Hohenberg. "Existence of long-range order in one and two dimensions". *Phys. Rev.* **158** (1967), 383.

[33] M. Inguscio, S. Stringari, and C. Wieman, eds. *Bose–Einstein condensation in atomic gases*. Italian Physical Society, 1999.

[34] R. Jastrow. "Many-body problem with strong forces". *Phys. Rev.* **98** (1955), 1479–1484.

[35] N. N. Khuri, A. Martin, J.-M. Richard, and T. T. Wu. "Low-energy potential scattering in two and three dimensions". *J. Math. Phys.* **50** (2009), 072105.

[36] J. M. Kosterlitz. "The critical properties of the two-dimensional *xy* model". *J. Phys. C* **7** (1974), 1046.

[37] J. M. Kosterlitz and D. J. Thouless. "Ordering, metastability and phase transitions in two-dimensional systems". *J. Phys. C* **6** (1973), 1181.

[38] B. Landon and R. Seiringer. "The scattering length at positive temperature". *Lett. Math. Phys.* **100** (2012), 237–243.

[39] T. D. Lee and C. N. Yang. "Many-body problem in quantum mechanics and quantum statistical mechanics". *Phys. Rev.* **105** (1957), 1119–1120; T. D. Lee, K. Huang, and C. N. Yang. "Eigenvalues and eigenfunctions of a Bose system of hard spheres and its low-temperature properties". *Phys. Rev.* **106** (1957), 1135–1145.

[40] A. J. Leggett. "Bose–Einstein condensation in the alkali gases: some fundamental concepts". *Rev. Mod. Phys.* **73** (2001), 307.

[41] M. Lewin, P. T. Nam, S. Serfaty, and J. P. Solovej. “Bogoliubov spectrum of interacting Bose gases”. *Comm. Pure Appl. Math.* **68** (2015), 413–471.

[42] E. H. Lieb. “Simplified approach to the ground state energy of an imperfect Bose gas”. *Phys. Rev.* **130** (1963), 2518–2528.

[43] E. H. Lieb. “The Bose fluid”. *Lecture notes in theoretical physics VIIC*. Ed. by W. E. Brittin. Univ. of Colorado Press, 1964, 175–224.

[44] E. H. Lieb. “The classical limit of quantum spin systems”. *Comm. Math. Phys.* **31** (1973), 327–340.

[45] E. H. Lieb, R. Seiringer, and J. P. Solovej. “Ground-state energy of the low-density Fermi gas”. *Phys. Rev. A* **71** (2005), 053605.

[46] E. H. Lieb, R. Seiringer, J. P. Solovej, and J. Yngvason. *The mathematics of the Bose gas and its condensation*. Oberwolfach Seminars, Vol. **34**. Basel, Boston, Berlin: Birkhäuser, 2005.

[47] E. H. Lieb, R. Seiringer, and J. Yngvason. “Bosons in a trap: a rigorous derivation of the Gross-Pitaevskii energy functional”. *Phys. Rev. A* **61** (2000), 043602.

[48] E. H. Lieb, R. Seiringer, and J. Yngvason. “Justification of c-number substitutions in bosonic Hamiltonians”. *Phys. Rev. Lett.* **94** (2005), 080401.

[49] E. H. Lieb and J. P. Solovej. “Ground state energy of the one-component charged Bose gas”. *Comm. Math. Phys.* **217** (2001), 127–163.

[50] E. H. Lieb and J. P. Solovej. “Ground state energy of the two-component charged Bose gas”. *Comm. Math. Phys.* **252** (2001), 485–534.

[51] E. H. Lieb and J. Yngvason. “Ground state energy of the low density Bose gas”. *Phys. Rev. Lett.* **80** (1998), 2504–2507.

[52] E. H. Lieb and J. Yngvason. “The ground state energy of a dilute two-dimensional Bose gas”. *J. Stat. Phys.* **103** (2001), 509–526.

[53] L. Liu and K. W. Wong. “Bose system of hard spheres”. *Phys. Rev.* **132** (1963), 1349.

[54] S. Mayer and R. Seiringer. “The free energy of the two-dimensional dilute Bose gas. II. Upper bound” (2020), in preparation.

[55] N. D. Mermin and H. Wagner. “Absence of ferromagnetism or Antiferromagnetism in one- or two-dimensional isotropic Heisenberg models”. *Phys. Rev. Lett.* **17**.22 (1966), 1133–1136.

[56] P. T. Nam and R. Seiringer. “Collective excitations of Bose gases in the mean-field regime”. *Arch. Ration. Mech. Anal.* **215** (2015), 381–417.

[57] M. Napiórkowski, R. Reuvers, and J. P. Solovej. “The Bogoliubov free energy functional II: the dilute limit”. *Comm. Math. Phys.* **360** (2017), 347–403.

[58] M. Napiórkowski, R. Reuvers, and J. P. Solovej. “Calculation of the critical temperature of a dilute Bose gas in the Bogoliubov approximation”. *Europhys. Lett.* **121** (2018), 10007.

[59] M. Napiórkowski, R. Reuvers, and J. P. Solovej. “The Bogoliubov free energy functional I: existence of minimizers and phase diagram”. *Arch. Ration. Mech. Anal.* **229** (2018), 1037–1090.

[60] M. Ohya and D. Petz. *Quantum entropy and its use*. Texts and monographs in physics. Berlin, Heidelberg: Springer, 2004.

[61] A. A. Ovchinnikov. “On the description of a two-dimensional Bose gas at low densities”. *J. Phys. Condens. Matter* **5** (1993), 8665–8676.

[62] C. Pethick and H. Smith. *Bose–Einstein condensation of dilute gases*. Cambridge University Press, 2001.

[63] L. P. Pitaevskii and S. Stringari. *Bose–Einstein condensation*. Oxford University Press, 2003.

[64] V. N. Popov. *Functional integrals in quantum field theory and statistical physics*. Dordrecht: Reidel, 1983.

[65] D. W. Robinson. *The thermodynamic pressure in quantum statistical mechanics*. Berlin, Heidelberg, New York: Springer-Verlag, 1971.

[66] D. Ruelle. *Statistical mechanics: rigorous results*. Reading, Massachusetts: W. A. Benjamin, Inc., 1969.

[67] M. Schick. “Two-dimensional system of hard core bosons”. *Phys. Rev. A* **3** (1971), 1067–1073.

[68] R. Seiringer. “A correlation estimate for quantum many-body systems at positive temperature”. *Rev. Math. Phys.* **18** (2006), 233–253.

[69] R. Seiringer. “The thermodynamic pressure of a dilute Fermi gas”. *Comm. Math. Phys.* **261** (2006), 729–758.

[70] R. Seiringer. “Free energy of a dilute Bose gas: lower bound”. *Comm. Math. Phys.* **279** (2008), 595–636.

[71] R. Seiringer. “The excitation spectrum for weakly interacting bosons”. *Comm. Math. Phys.* **306** (2011), 565–578.

[72] R. Seiringer. “Hot topics in cold gases”. *Japan. J. Math.* **8** (2013), 182–232.

[73] R. Seiringer and D. Ueltschi. “Rigorous upper bound on the critical temperature of dilute Bose gases”. *Phys. Rev. B* **80** (2009), 014502.

[74] B. Simon. “The bound state of weakly coupled Schrödinger operators in one and two dimensions”. *Annals of Physics* **97** (1975), 279–288.

[75] J. P. Solovej. “Upper bounds to the ground state energies of the one- and two-component charged Bose gases”. *Comm. Math. Phys.* **266** (2006), 797–818.

[76] J. R. Taylor. *Scattering theory: the quantum theory on nonrelativistic collisions*. John Wiley & Sons, 1972.

[77] T. T. Wu. “Ground state of a Bose system of hard spheres”. *Phys. Rev.* **115** (1959), 1390.

[78] H.-T. Yau and J. Yin. “The second order upper bound for the ground energy of a Bose gas”. *J. Stat. Phys.* **136** (2009), 453–503.

[79] J. Yin. “Free energies of dilute Bose gases: upper bound”. *J. Stat. Phys.* **141** (2010), 683–726.

[80] V. I. Yukalov. “Principal problems in Bose–Einstein condensation of dilute gases”. *Laser Phys. Lett.* **1** (2004), 435–461.

[81] V. A. Zagrebnov and J. B. Bru. “The Bogoliubov model of weakly interacting Bose gas”. *Phys. Reports* **350** (2001), 291–434.