The Ground State Energy of a Dilute Bose Gas in Dimension $n > 3$

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Abstract

We consider a Bose gas in spatial dimension $n > 3$ with a repulsive, radially symmetric two-body potential $V$. In the limit of low density $\rho$, the ground state energy per particle in the thermodynamic limit is shown to be $(n - 2)|S^{n-1}|a^{n-2}\rho$, where $|S^{n-1}|$ denotes the surface measure of the unit sphere in $\mathbb{R}^n$ and $a$ is the scattering length of $V$. Furthermore, for smooth and compactly supported two-body potentials, we derive upper bounds to the ground state energy with a correction term $(1 + C\gamma)8\pi^2a^6\rho^2|\ln(a^4\rho)|$ in dimension $n = 4$, where $\gamma := \int V(x)|x|^{-2} \, dx$, and a correction term which is $O(\rho^2)$ in higher dimensions.

1 Introduction

The experimental realization of Bose-Einstein Condensation in 1995 [1] has inspired renewed interest in a rigorous understanding of the interacting Bose gas, and in particular the ground state energy. The typical model for the energy of $N$ bosons enclosed in a box $\Lambda = \Lambda_L := (-L/2, L/2)^n$, is the Hamiltonian

$$H_{N,L} = \sum_{i=1}^N -\Delta_i + \sum_{1 \leq j < k \leq N} V(x_j - x_k)$$

on $L^2_{\text{sym}}(\Lambda^n)$ (the set of totally symmetric $L^2$-functions on $\Lambda^n$). Here units are chosen such that $\hbar^2/2m = 1$, where $m$ is the mass of a particle. We will always assume that the two-body potential $V$ is a nonnegative and radially symmetric function on $\mathbb{R}^n$. Let

$$E_0(N, L) := \inf \sigma(H_{N,L}) = \inf \{\langle \Psi, H_{N,L} \Psi \rangle : \|\Psi\| = 1\}$$

denote the ground state energy of the Bose gas, and let

$$e_0(\rho) := \lim_{N \to \infty} \frac{E_0(N, (N/\rho)^{1/n})}{N}$$

(1.2)
denote the ground state energy per particle in the thermodynamic limit at density $\rho > 0$. The latter is independent of whatever boundary conditions imposed on $\Lambda$. We let $a$ denote the scattering length of $V$ (see section 2) and note that $Y := a^n \rho$ is a dimensionless quantity.

In dimension $n = 3$, the asymptotic behavior of $e_0(\rho)$ in the limit of low density was studied by Bogoliubov [2], Lee-Yang [9] and Lee-Huang-Yang [8] in the 1940-50’s. In particular, the latter applied the pseudopotential method to derive the expansion

$$e_0(\rho) = 4\pi a \rho \left( 1 + \frac{128}{15\sqrt{\pi}} Y^{1/2} + o(Y^{1/2}) \right)$$

as $Y \to 0$, now known as the Lee-Huang-Yang formula (LHY). To give a mathematical proof of LHY is still an open problem, except in a special case of $\rho$ in a so-called simultaneously weak coupling and high density regime, and for a rather narrow class of potentials [6]. Even to prove the leading order term in LHY turned out to be a hard problem: A variational calculation carried out by Dyson in 1957 [3] showed the upper bound

$$e_0(\rho) \leq 4\pi a \rho (1 + CY^{1/3})$$

for hard-core interactions. This has later been generalized to general nonnegative, radially symmetric potentials [12]. However, no proof of a matching, leading order lower bound was available until 1998, where Lieb-Yngvason managed to show that $e_0(\rho) \geq 4\pi a \rho (1 - CY^{1/17})$. Their approach was improved in [7] to yield $e_0(\rho) \geq 4\pi a \rho (1 - C\rho^{1/3} \ln(\rho))$. At the present time, no lower bound has captured even the correct order in the expansion parameter $Y$ in LHY. For the upper bound there has been success though: In [4] a trial state of the form

$$\Psi = \exp \left( \frac{1}{2} \sum_{p \neq 0} c_p a_p^+ a_{-p} + \sqrt{N_0} a_0^+ \right) |0\rangle$$

was used to derive an upper bound

$$e_0(\rho) \leq 4\pi a \rho \left( 1 + \frac{128}{15\sqrt{\pi}} (1 + C\lambda) Y^{1/2} \right) + C\rho^{2} \ln \rho,$$

for a coupled two-body potential $V = \lambda \tilde{V}$. While the correction term has the correct order in $Y$, the constant is only correct in the limit of weak coupling, $\lambda \to 0$. The (Fock) trial state (1.3) is inspired by the Bogoliubov approximation, and the crucial feature is that particles of nonzero momenta appear only in pairs of opposite momenta. Similar states have previously been considered by Girardeau-Arnowitt [5] and Solovej [20] in the context of Bose gases. In a paper from 2009 [22] Yau-Yin introduced a new trial state, extending the properties of (1.3). More precisely, they include pairs with total momentum of order $\rho^{1/2}$ (however their trial state has a fixed number of particles in contrast to 1.3). This turns out to lower the energy significantly and their result is an upper bound consistent with LHY. We note however that the calculation with the Yau-Yin trial state is somewhat more involved than the computation with (1.3).

The model (1.1) has also been studied in other dimensions. The case $n = 1$ (with a delta-function potential) was already considered back in 1963 by Lieb-Liniger [11] and turned out to be exactly solvable. In two dimensions, the leading order term was, to our knowledge, first identified by Schick [18] in 1971 to be $4\pi \rho \ln(a^2 \rho)^{-1}$. This was
rigorously proven to be correct by Lieb-Yngvason in 2001 [14]. To our knowledge there are yet no rigorous results on the 2-dimensional correction term (in fact, it seems that there is not even consensus about what this term should be: compare e.g. [18], [21] and [15]). In [21] Yang reexamined the pseudopotential method in dimension two, four and five. In the latter he found the method inconclusive, while in four dimensions he derived the expansion
\[
e_0(\rho) = 4\pi^2a^2\rho[1 + 2\pi^2Y|\ln Y| + o(Y\ln Y)] \quad \text{as } Y \to 0.
\] (1.4)
We remark that in Yangs paper the correction $2\pi^2Y|\ln Y|$ appears to be $4\pi^2Y|\ln Y|$, due to a minor miscalculation.

In this paper we test some of the rigorous 3-dimensional calculations in higher dimensions. We follow the proofs of Dyson and Lieb-Yngvason to obtain the $n$-dimensional upper- and lower bounds (Theorem 2.2 and Theorem 2.3),
\[
1 - CY^\alpha \leq \frac{e_0(\rho)}{s_na^{n-2}\rho} \leq 1 + CY^\beta,
\] (1.5)
where $s_n := (n-2)|S^{n-1}|$, $|S^{n-1}|$ denotes the surface measure of the unit sphere in $\mathbb{R}^n$ and where
\[
\alpha = \frac{n-2}{n(n+2)+2} \quad \text{and} \quad \beta = \frac{n-2}{n}.
\]
Secondly, we employ the trial state (1.3) to improve the upper bounds. In dimension $n = 4$ we show that (Theorem 3.1)
\[
e_0(\rho) \leq 4\pi^2a^2\rho[1 + 2\pi^2(1 + C\gamma Y|\ln Y|) + O(\rho^2)],
\]
where $\gamma := \int V(x)|x|^{-2}dx$, consistent with (1.4) in the limit $\gamma \to 0$. In dimension $n \geq 5$ the calculation yields the upper bound (Theorem 3.1)
\[
e_0(\rho) \leq s_na^{n-2}\rho + O(\rho^2).
\]
The second order asymptotics of $e_0(\rho)$ becomes more subtle in dimension $n > 3$. The correction to the energy is given in terms of certain integrals, which, in three dimensions, are exactly computable in the limit $\rho \to 0$, in a straight-forward manner. This is not the case in higher dimensions, and a more careful analysis has to be carried out. In dimension $n \geq 5$ we have not been able to identify the expansion parameter $Y$ in the correction term, nor an explicit coefficient.

Finally, since (1.3) is a Fock state, we need the fact that the canonical ground state energy defined in (1.2) can be recovered from the grand-canonical setting. Although this is a well-known result, we did not come across a good reference for it, and hence we have included a proof in Appendix A.

2 The Leading Order Term

In this section we prove the upper and lower bounds in (1.5). We will assume that $V$ is a nonnegative, radial and measurable function on $\mathbb{R}^n$, where $n \geq 3$. The scattering length
of $V$ is denoted by $a$ and may be defined via the variational problem (see e.g. [10], [23])
\[
s_n a^{n-2} := \inf_u \int_{\mathbb{R}^n} |\nabla u|^2 + \frac{1}{2} Vu^2,
\]
where the infimum is taken over all nonnegative, radially symmetric functions $u \in H^1_{\text{loc}}(\mathbb{R}^n)$ satisfying $u(r) \to 1$ as $r \to \infty$. Notice that such functions are automatically continuous away from the origin. Also, it is easy to see that we may restrict attention to radially increasing functions. Moreover, we remark that $a$ is finite if and only if $V$ is integrable at infinity. In many cases the infimum in (2.1) is a unique minimum, and the minimizer $u$ satisfies the zero-energy scattering equation
\[
-\Delta u + \frac{1}{2} V u = 0
\]
in the sense of distributions on $\mathbb{R}^n$. The existence of a scattering solution for a nonnegative, radially symmetric and compactly supported potential is established in [14]. We note briefly some properties of the scattering solution $u$, referring to [14], [10] for details:

(i) For large $r$, $u(r) \approx 1 - (a/r)^{n-2}$, or more precisely
\[
\lim_{r \to \infty} \frac{1 - u(r)}{(a/r)^{n-2}} = 1.
\]
In fact
\[
u(r) \geq 1 - (a/r)^{n-2},
\]
with equality for $r > R_0$ if $\text{supp}(V) \subset B(0,R_0)$.

(ii) Monotonicity: If $V \leq \tilde{V}$, then $a \leq \tilde{a}$, while $u \geq \tilde{u}$.

(iii) Regularity imposed on $V$ is inherited by $u$. For instance, one may apply elliptic regularity and Sobolev imbedding’s to show that if $V$ is smooth, so is $u$.

(iv) For $V \in L^1(\mathbb{R}^n)$, it follows from (2.2) that $u$ can be represented as
\[
1 - u(x) = \frac{1}{2} \Gamma(Vu)(x) := \frac{1}{2s_n} \int_{\mathbb{R}^n} V(y)u(y) \frac{|x - y|^{n-2}}{dy}.
\]

By (2.3) and the dominated convergence theorem it then follows that
\[
2s_n a^{n-2} = \int_{\mathbb{R}^n} V(x)u(x) \, dx.
\]

The main result of this section is the following, which is an immediate consequence of Theorem 2.2 and Corollary 2.10 below.

**Theorem 2.1.** Let $n \geq 3$ and suppose that $V$ is nonnegative, radially symmetric, measurable and decays faster than $r^{-\nu}$ at infinity, where $\nu = (6n-2)/5$. Suppose furthermore that $V$ admits a scattering solution. Then
\[
\lim_{\rho \to 0} \frac{\epsilon_0(\rho)}{s_n a^{n-2} \rho} = 1.
\]
2.1 The Upper Bound

We have the following dimensional generalization of [3], [10].

**Theorem 2.2.** Let \( n \geq 3 \) and suppose that \( V \) is nonnegative, radially symmetric and measurable.

(i) Without further assumptions,
\[
\limsup_{\rho \to 0} \frac{e_0(\rho)}{s_n a_n^{-2} \rho} \leq 1.
\]

(ii) There exist \( C, \delta > 0 \) independent of \( V \) such that, if \( V \) admits a scattering solution, then
\[
e_0(\rho) \leq s_n a_n^{-2} \rho \left[ 1 + CY^{1-2/n} \right],
\]
whenever \( Y \leq \delta \).

**Proof.** We employ the periodic trial state of Dyson [3]. This state is not symmetric, but since the ground state of \( H_{N,L} \) on the full space \( L^2(\Lambda N) \) is symmetric [10], we obtain an upper bound to \( e_0(\rho) \). Suppose that \( u \in H^1_{\text{loc}}(\mathbb{R}^n) \) is nonnegative, radially symmetric, increasing and moreover that \( u(r) \to 1 \) as \( r \to \infty \). The trial state is then defined by
\[
\Psi := F_2 \cdot F_3 \cdots F_N,
\]
where
\[
F_i := \min_{1 \leq j < i} \left[ \min_{m \in \mathbb{Z}} f(x_i - x_j - mL) \right]
\]
and
\[
f(r) := \begin{cases} 
\frac{u(r)}{u(b)} & 0 \leq r \leq b \\
1 & r > b
\end{cases}
\]
for some (large) \( b > 0 \) to be chosen. Following the calculation in [10] we obtain
\[
e_0(\rho) \leq \frac{J \rho + \frac{2}{3} (K \rho)^2}{(1 - I \rho)^2},
\]
(2.8)
where
\[
I := \int (1 - f(x)^2) \, dx, \quad K := \int f(x) |\nabla f(x)| \, dx
\]
and
\[
J := \int |\nabla f(x)|^2 + \frac{1}{2} V(x) f(x)^2 \, dx.
\]
It follows that
\[
\limsup_{\rho \to 0} \rho e_0(\rho) \rho^{-1} \leq J \leq \frac{1}{u(b)^2} \int |\nabla u(x)|^2 + \frac{1}{2} V(x) u(x)^2 \, dx,
\]
where we have used
\[
f(r) \leq \frac{u(r)}{u(b)} \quad \text{and} \quad f'(r) \leq \frac{u'(r)}{u(b)}
\]
in the latter inequality. In the limit $b \to \infty$ we get

$$\limsup_{\rho \to 0} e_0(\rho) \rho^{-1} \leq \int |\nabla u(x)|^2 + \frac{1}{2} V(x) u(x)^2 \, dx,$$

and minimizing over $u$ yields (i), by definition of the scattering length.

In case $V$ admits a scattering solution, we apply the above construction with $u$ being this particular function. The bound (2.4) then allows us to estimate more explicitly. Indeed, we have

$$f(r) \geq \left[ 1 - \left( \frac{a}{r} \right)^{n-2} \right] + \frac{1}{n-2},$$

and hence

$$I \leq |S^{n-1}| \left( \int_0^a r^{-1} \, dr + \int_a^b 2a^{n-2} r \, dr \right) \leq |S^{n-1}| a^{n-2} b^2.$$

Next,

$$J \leq \frac{s_n a^{n-2}}{u(b)^2} \leq \frac{s_n a^{n-2}}{(1 - (a/b)^{n-2})^2},$$

provided $b > a$. Finally, using $f(r) \leq 1$ and an integration by parts yields

$$K \leq |S^{n-1}| \int_0^b f'(r) r^{-1} \, dr \leq |S^{n-1}| \left( b^{n-1} - (n - 1) \int_0^b f(r) r^{-2} \, dr \right).$$

However,

$$\int_0^b f(r) r^{-2} \, dr \geq \int_a^b \left[ 1 - (a/r)^{n-2} \right] r^{-2} \, dr$$

$$= \frac{b^{n-1}}{n-1} - a^{-2} b + \frac{n-2}{n-1} a^{n-1} \geq \frac{b^{n-1}}{n-1} - a^{n-2} b,$$

and hence $K \leq |S^{n-1}| (n - 1) a^{n-2} b$. Now, by choosing $b := (|S^{n-1}| \rho)^{-1/n}$, we have

$$(a/b)^{n-2} = |S^{n-1}| a^{n-2} b^2 \rho = \tilde{Y} \beta,$$

where $\tilde{Y} := |S^{n-1}| Y$ and $\beta := (n - 2)/n$. Note that in particular $b > a$ if $\tilde{Y} < 1$. In total we have

$$e_0(\rho) \leq s_n a^{n-2} \rho \left[ \frac{1}{(1 - \tilde{Y} \beta)^4} + \frac{C Y \beta}{(1 - \tilde{Y} \beta)^2} \right] \leq s_n a^{n-2} \rho (1 + \tilde{C} Y \beta),$$

provided $\tilde{Y}$ is bounded away from 1.

\[ \square \]

### 2.2 The Lower Bound

In this section we prove an $n$-dimensional lower bound by following the steps in [13]. The assumption of compact support in Theorem 2.3 below is relaxed in Corollary 2.10.

**Theorem 2.3.** Let $n \geq 3$ and suppose that $V$ is nonnegative, radially symmetric, measurable and compactly supported with, say, $\text{supp}(V) \subset B(0,R_0)$. There exist $C, \delta > 0$ independent of $V$ such that

$$e_0(\rho) \geq s_n a^{n-2} \rho (1 - CY \alpha),$$
where
\[ \alpha := \frac{n-2}{n(n+2)+2}, \]  
(2.9)

provided
\[ Y \leq \min \{ \delta, (a/R_0)^{\alpha/2} \}. \]  
(2.10)

In order to prove Theorem 2.3 we consider \( H = H_{N,L} \) with Neumann boundary conditions on \( \Lambda \). The first step is to obtain an \( n \)-dimensional version of Dyson’s lemma. In what follows we set \( a_n := (n-2)a^{n-2} \).

**Lemma 2.4 (Dyson’s Lemma).** Assume that \( U \) is a measurable, nonnegative and radially symmetric function on \( \mathbb{R}^n \), which satisfies
\[ U(r) = 0, \quad \text{for } r \leq R_0, \quad \text{and } \int_0^\infty U(r)r^{n-1}dr \leq 1. \]

Let \( B \subseteq \mathbb{R}^n \) be open and star shaped w.r.t. the origin. Then
\[ \int_B |\nabla \varphi(x)|^2 + \frac{1}{2}V(x)|\varphi(x)|^2 \, dx \geq a_n \int_B U(x)|\varphi(x)|^2 \, dx, \]
for each \( \varphi \in H^1(B) \).

**Proof.** For any \( \omega \in \mathbb{S}^{n-1} \) we let
\[ R(\omega) = \sup\{ r \geq 0 : s\omega \in B, \text{ for each } 0 \leq s \leq r \} \]
denote the (possibly infinite) distance from the origin to the boundary of \( B \) in the direction of \( \omega \). Since \( B \) is open and star shaped w.r.t. the origin, it follows that, for any \( r \geq 0 \), \( r\omega \in B \) if and only if \( r < R(\omega) \). By passing into polar coordinates, we then see that it suffices to show that, for each fixed \( \omega \in \mathbb{S}^{n-1} \),
\[ \int_0^{R(\omega)} \left( |f'(r)|^2 + \frac{1}{2}V(r)|f(r)|^2 \right) r^{n-1} \, dr \geq a_n \int_0^{R(\omega)} U(r)|f(r)|^2 \, r^{n-1} \, dr, \]
(2.11)

where \( f(r) := \varphi(r\omega) \) with \( |f(r)| \leq |\nabla \varphi(r\omega)| \). We may assume that \( R(\omega) > R_0 \), since otherwise the right hand side in (2.11) vanishes, and we claim that
\[ \int_0^{R(\omega)} \left( |f'(r)|^2 + \frac{1}{2}V(r)|f(r)|^2 \right) r^{n-1} \, dr \geq a_n |f(R)|^2, \]
(2.12)

for each \( R_0 < R < R(\omega) \). Indeed, if \( f(R) \neq 0 \), then the function \( u \) given by \( u(x) = |f(|x|)/f(R)| \) for \( |x| \leq R \) and \( u(x) = 1 \) for \( |x| > R \) is admissible in (2.1), and since \( V(r) = 0 \), for \( r > R \), it follows that
\[ s_n a^{n-2} \leq \frac{|\mathbb{S}^{n-1}|}{|f(R)|^2} \int_0^{R(\omega)} \left( |f'(r)|^2 + \frac{1}{2}V(r)|f(r)|^2 \right) r^{n-1} \, dr. \]

Now (2.11) follows by multiplying both sides of (2.12) with \( U(R)R^{n-1} \) and then integrating w.r.t. \( R \).
Corollary 2.5. Suppose that $U$ satisfies the conditions of Lemma 2.4 and define

$$W := \sum_{i=1}^{N} U \circ t_i, \quad t_i(x_1, \ldots, x_N) := \min_{j \neq i} |x_i - x_j|.$$ 

Then $H \geq a_n W$.

Proof. Since $V$ is nonnegative and radial,

$$\sum_{i=1}^{N} V(t_i(\vec{x})) \leq \sum_{i=1}^{N} \sum_{j \neq i} V(x_i - x_j) + \sum_{i=1}^{N} \sum_{j > i} V(x_i - x_j) = 2 \sum_{i < j} V(x_i - x_j),$$

for each $\vec{x} = (x_1, \ldots, x_N)$, and hence

$$H \geq \sum_{i=1}^{N} (- \Delta_i + \frac{1}{2} V \circ t_i). \quad (2.13)$$

We focus on the first term $i = 1$, and fix $x_2, \ldots, x_N \in \Lambda$. For $j \neq 1$ define

$$B_j = \{ x_1 \in \Lambda : t_1(\vec{x}) = |x_1 - x_j| \}.$$ 

Fix an arbitrary $\psi \in H^1(\Lambda^N)$. By a change of variables $x_1 \mapsto x_1 + x_j$, and by noting that $(B_j - x_j)$ is star shaped w.r.t. the origin (indeed convex), we may apply Dyson’s lemma to obtain

$$\int_{B_j} |\nabla_1 \psi(\vec{x})|^2 + \frac{1}{2} V(t_1(\vec{x}))|\psi(\vec{x})|^2 \, dx_1 \geq a_n \int_{B_j} U(t_1(\vec{x}))|\psi(\vec{x})|^2 \, dx_1, \quad (2.14)$$

for each $j \neq 1$. Moreover, since the $B_j$’s cover $\Lambda$ disjointly (a.e.), we conclude that [2.14] holds with $B_j$ replaced by $\Lambda$. Then, by Fubini’s theorem,

$$\int_{\Lambda^N} |\nabla_1 \psi(\vec{x})|^2 + \frac{1}{2} V(t_1(\vec{x}))|\psi(\vec{x})|^2 \, d\vec{x} \geq a_n \int_{\Lambda^N} U(t_1(\vec{x}))|\psi(\vec{x})|^2 \, d\vec{x}.$$ 

We get analogous contributions from $i = 2, \ldots, N$ in (2.13), and upon adding them, we obtain the result. \qed

We now combine Corollary 2.5 with Temple’s inequality [16] in a perturbative approach. The parameters $R$ and $\varepsilon$ appearing below will be chosen appropriately later on.

Lemma 2.6. Let $0 < \varepsilon < 1$ and $R_0 < R < L/2$. Suppose that

$$G(N, L) := \varepsilon \pi^2 L^2 - s_n a^{n-2} L^{-n} N^2 > 0.$$ 

Then

$$E_0(N, L) \geq N(N-1) K(N, L),$$

where

$$K(N, L) := \frac{s_n a^{n-2}}{L^n} (1 - \varepsilon) (1 - 2R/L)^N \left(1 - v_n \frac{R^n}{L^n}ight)^{N-2} \left(1 - \frac{n(n-2)a^{n-2}N}{(R^n - R_0^n)G(N, L)}\right).$$

Here $v_n$ denotes the measure of the unit ball in $\mathbb{R}^n$. 

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Proof. Suppose that $U$ and $W$ are as in Lemma 2.4 respectively Corollary 2.5. Together with the fact that $V$ is nonnegative, we then have a lower bound

$$H = \varepsilon H + (1 - \varepsilon) H \geq -\varepsilon \Delta + (1 - \varepsilon) a_n W =: \tilde{H},$$

and consequently

$$E_0(N, L) \geq \tilde{E}_0(N, L) := \inf \sigma(\tilde{H}). \tag{2.15}$$

We estimate $\tilde{E}_0(N, L)$ by employing Temple’s inequality in the ground state of $-\varepsilon \Delta$ (with Neumann Boundary conditions), which is the constant function $\varphi_0(x) \equiv |\Lambda|^{-N/2}$ with corresponding eigenvalue zero. Given any operator $A$ on $L^2(\Lambda^N)$ with domain containing $\varphi_0$, we let $\langle A \rangle = \langle \varphi_0, A \varphi_0 \rangle$. Temple’s inequality and (2.15) yields

$$E_0(N, L) \geq \langle \tilde{H} \rangle - \langle \tilde{H}^2 \rangle - \langle \tilde{H} \rangle^2 / \tilde{E}_1 - (1 - \varepsilon) a_n \langle W \rangle,$$

provided $\langle \tilde{H} \rangle < \tilde{E}_1$, where $\tilde{E}_1$ is the second lowest eigenvalue of $\tilde{H}$. Note however that, since $W$ is nonnegative, we have $\tilde{H} \geq -\varepsilon \Delta$, and hence $\tilde{E}_1 \geq \varepsilon \pi^2 / L^2$, which is the second lowest eigenvalue of $-\varepsilon \Delta$. We now choose the function $U$ to be

$$U(r) := \begin{cases} 
  n(R^n - R_0^n)^{-1} & \text{for } R_0 < r < R \\
  0 & \text{otherwise}
\end{cases}.$$

By discarding the term $\langle W \rangle^2$, replacing $(1 - \varepsilon)$ by 1 in two appropriate places and employing the fact that

$$\langle W^2 \rangle \leq n \cdot N(R^n - R_0^n)^{-1} \langle W \rangle,$$

we obtain

$$E_0(N, L) \geq (1 - \varepsilon) a_n \langle W \rangle \left[ 1 - \frac{na_n N}{(R^n - R_0^n)(\varepsilon \pi^2 / L^2 - a_n \langle W \rangle)} \right], \tag{2.16}$$

provided $a_n \langle W \rangle < \varepsilon \pi^2 / L^2$. To estimate this further, we need upper and lower bounds on $\langle W \rangle$, and we claim that

$$\frac{|S^{n-1}|}{L^n} N(N - 1)(1 - 2R/L)^n(1 - v_n R^n / L^n)^{N-2} \leq \langle W \rangle \leq \frac{|S^{n-1}|}{L^n} N(N - 1). \tag{2.17}$$

This will conclude the proof of the lemma. For the upper bound in (2.17) we fix $x_1 \in \Lambda$ and notice that

$$\{(x_2, \ldots, x_N) \in \Lambda^{N-1} : R_0 < t_1(x) < R \} \subseteq \bigcup_{j=2}^N F_j,$$
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where \( \vec{x} = (x_1, \ldots, x_N) \) and \( F_j = \Lambda^{N-1} \), except that the \( j \)'th factor is replaced by \( B(x_1, R) \setminus B(x_1, R_0) \). It follows that

\[
\int_{\Lambda^{N-1}} U(t_1(\vec{x})) \, dx_2 \ldots dx_N \leq \frac{n}{R^n - R_0^n} \sum_{j=2}^{N} |F_j| = |S^{n-1}|((N-1)|\Lambda|)^{N-2}.
\]

By integrating over \( x_1 \in \Lambda \) and then adding the identical contributions from the integrals of \( U(t_2), \ldots, U(t_N) \), we arrive at the upper bound in (2.17). To verify the lower bound, we let \( \Lambda' \subseteq \Lambda \) denote the cube with same center as \( \Lambda \) but with side length \( L - 2R \). Fix \( x_1 \in \Lambda' \) and notice that \( B(x_1, R) \subseteq \Lambda \). We then have

\[
\bigcup_{j=2}^{N} E_j \subseteq \{(x_2, \ldots, x_N) \in \Lambda^{N-1} : R_0 < t_1(\vec{x}) < R\}, \tag{2.18}
\]

where

\[
E_j = (\Lambda \setminus B(x_1, R))^{N-1}
\]

except again that the \( j \)'th factor is replaced by \( B(x_1, R) \setminus B(x_1, R_0) \). Since the \( E_j \)'s are pairwise disjoint, (2.18) implies that

\[
\int_{\Lambda^{N-1}} U(t_1(\vec{x})) \, dx_2 \ldots dx_N \geq \frac{n}{R^n - R_0^n} \sum_{j=2}^{N} |E_j| = |S^{n-1}|((N-1)(|\Lambda| - v_n R^n))^{N-2},
\]

and integrating over \( \Lambda \supset \Lambda' \ni x_1 \), we obtain

\[
\int_{\Lambda^{N}} U(t_1(\vec{x})) \, d\vec{x} \geq |S^{n-1}|((N-1)(L - 2R)^n(|\Lambda| - v_n R^n))^{N-2}.
\]

Again, by adding identical contributions from the integrals of \( U(t_2), \ldots, U(t_N) \), we have proved (2.17) and with it the lemma.

Note that, for fixed \( \rho > 0 \)

\[
G(\rho L^n, L) \leq \pi^2 L^{-2} - s_n a^{n-2} \rho^2 L^n < 0,
\]

for large \( L \), so Lemma 2.6 may not immediately be applied to get estimates in the thermodynamic limit.

**Lemma 2.7.** The mapping \( N \mapsto E_0(N, L) \) is superadditive, i.e.,

\[
E_0(k + m, L) \geq E_0(k, L) + E_0(m, L), \quad \text{for all } k, m \in \mathbb{N}.
\]

**Proof.** Fix an arbitrary normalized \( \psi \in H^1(\Lambda^{k+m}) \). Since \( V \) is nonnegative, it follows that

\[
\langle \psi, H \psi \rangle \geq \int_{\Lambda^{k+m}} \sum_{i=1}^{k} |\nabla_i \psi|^2 + \sum_{1 \leq i < j \leq k} V(x_i - x_j)|\psi|^2 + \int_{\Lambda^{k+m}} \sum_{i=k+1}^{k+m} |\nabla_i \psi|^2 + \sum_{k+1 \leq i < j \leq k+m} V(x_i - x_j)|\psi|^2. \tag{2.19}
\]
Then, by Fubini’s theorem,
\[ \int_{\Lambda^{k+m}} \sum_{i=1}^{k} |\nabla_i \psi|^2 + \sum_{1 \leq i < j \leq k} V(x_i - x_j)|\psi|^2 \geq \int_{\Lambda^m} \left( E_0(k, L) \int_{\Lambda^k} |\psi|^2 \right) = E_0(k, L), \]
and similarly for the second term on the right-hand side in (2.19).

**Lemma 2.8.** Suppose that \( L/l \in \mathbb{N} \). Then
\[
E_0(N, L) \geq M \cdot \min \sum_{m=0}^{N} c_m E_0(m, l),
\]
where \( M := (L/l)^n \) and where the minimum is over all tuples \((c_0, \ldots, c_N)\) of numbers \(c_m \geq 0\) subject to the conditions
\[
\sum_{m=0}^{N} c_m = 1 \quad \text{and} \quad \sum_{m=0}^{N} mc_m = N/M. \tag{2.21}
\]

**Proof.** We partition \( \Lambda \) into \( M \) disjoint boxes \( \Lambda_1, \ldots, \Lambda_M \), each of side length \( l \). Correspondingly we have a partition \( \{\Omega_\beta\} \) of \( \Lambda^N \),
\[
\Omega_\beta := \Lambda_{\beta_1} \times \ldots \times \Lambda_{\beta_N}, \quad \beta = (\beta_1, \ldots, \beta_N), \quad 1 \leq \beta_j \leq M,
\]
and hence
\[
\langle \psi, H\psi \rangle = \sum_{\beta} \int_{\Omega_\beta} \sum_{i=1}^{N} |\nabla_i \psi|^2 + \sum_{i<j} V(x_i - x_j)|\psi|^2. \tag{2.22}
\]
Fix a \( \beta \) as above. By Fubini’s theorem, the integration regime \( \Omega_\beta \) may be replaced by \( \Lambda_{\alpha_1}^{\alpha_1} \times \ldots \times \Lambda_{\alpha_M}^{\alpha_M} \), for some multiindex \( \alpha \in \mathbb{N}_0^M \) with length \( |\alpha| = N \). For each \( 0 \leq m \leq N \), we let \( M \cdot c_m \) denote the number of components of \( \alpha \) equal to \( m \). By following the proof of Lemma 2.7, we split the kinetic energy into appropriate terms, and discard interactions between particles in different boxes to obtain the lower bound
\[
\int_{\Omega_\beta} \ldots \geq \left( \int_{\Omega_\beta} |\psi|^2 \right) \sum_{j=1}^{M} E_0(\alpha_j, l)
\]
\[
= \left( \int_{\Omega_\beta} |\psi|^2 \right) M \sum_{m=0}^{N} c_m E_0(m, l)
\]
\[
\geq \left( \int_{\Omega_\beta} |\psi|^2 \right) M \min \left( \sum_{m=0}^{N} c_m E_0(m, l) \right).
\]
Employing this estimate in (2.22) yields the result.

**Lemma 2.9.** Let \( \rho = N/L^n \). Suppose that \( L/l \in \mathbb{N} \), \( R_0 < R < l/2 \) and \( G(4\rho l^n, l) > 0 \). Then
\[
\frac{E_0(N, L)}{N} \geq (\rho l^n - 1)K(4\rho l^n, l).
\]
Proof. Suppose that \( c_m \geq 0 \) satisfies (2.21). We split the sum in (2.20) into two parts:

\[
\sum_m c_mE_0(m, l) = \sum_{m < p} c_mE_0(m, l) + \sum_{m \geq p} c_mE_0(m, l),
\]

for some \( p \in \mathbb{N} \) to be chosen. Suppose for now that \( G(p, l) > 0 \). Since \( G(N, L) \) and \( K(N, L) \) are decreasing functions of \( N \), Lemma 2.6 implies that

\[
E_0(m, l) \geq m(m - 1)K(p, l), \quad 0 \leq m \leq p,
\]

and hence

\[
\sum_{m < p} c_mE_0(m, l) \geq K(p, l)\sum_{m < p} c_mm(m - 1).
\]

Let \( t := \sum_{m < p} mc_m \). By the Cauchy-Schwarz inequality,

\[
t^2 \leq \left( \sum_{m < p} m^2 c_m \right) \left( \sum_{m < p} c_m \right) \leq \sum_{m < p} m^2 c_m,
\]

and it follows that

\[
\sum_{m < p} c_mm(m - 1) \geq t(t - 1).
\]

Thus we have

\[
\sum_{m < p} c_mE_0(m, l) \geq K(p, l)t(t - 1).
\]

We now employ the superadditivity of \( m \mapsto E_0(m, l) \) (Lemma 2.7) to obtain a lower bound on the second sum on the right hand side in (2.23). For \( m \geq p \) we write \( m = \lfloor m/p \rfloor p + r \), where \( \lfloor m/p \rfloor \) denotes the lower integer part of \( m/p \) and \( r \in \mathbb{N}_0 \) is the remainder. Notice that \( \lfloor m/p \rfloor \geq m/(2p) \) always. The superadditivity of \( E_0(m, l) \) then yields

\[
E_0(m, l) \geq m/(2p)E_0(p, l),
\]

and it follows that

\[
\sum_{m \geq p} c_mE_0(m, l) \geq \frac{E_0(p, l)}{2p}(k - t) \geq \frac{1}{2}(p - 1)(k - t)K(p, l),
\]

where \( k := N/M = \rho l^n \). Altogether we have

\[
\sum_{m=0}^{N} c_mE_0(m, l) \geq K(p, l)[t(t - 1) + \frac{1}{2}(p - 1)(k - t)].
\]

The choice \( p = \lfloor 4k \rfloor \) implies that \( x \mapsto (x(x - 1) + \frac{1}{2}(p - 1)(k - x)) \) is decreasing on \([0, k]\), which is where \( t \) lies, and hence the minimum is taken at \( x = k \). Thus we have that

\[
\frac{E_0(N, L)}{N} \geq \frac{1}{l^n} \sum_m c_mE_0(m, l) \geq K(p, l)(k - 1),
\]

as claimed. \( \square \)
We can now finish the proof of Theorem 2.3.

Proof of Theorem 2.3. Suppose that the conditions of Lemma 2.9 are satisfied. Recall that $Y = a^n \rho$. Then

\[
\frac{E_0(N, L)}{N} \geq s_n a^{n-2} \rho (1 - \varepsilon) (1 - 2nR/l) \left[ 1 - Y^{-1} (a/l)^n \right] \times \left[ 1 - 4v_n Y (l/a)^n (R/l)^n \right] \left[ 1 - \frac{4n(n - 2)l^n Y}{(R^n - R_0^n)(\varepsilon n^2 (a/l)^2 - 16s_n Y^2 (l/a)^n)} \right].
\]

We now make the ansatz

\[
\varepsilon = Y^\alpha, \quad a/l = Y^\beta, \quad \frac{R^n - R_0^n}{l^n} = Y^\gamma,
\]

for exponents $\alpha, \beta, \gamma > 0$. In particular this implies that

\[
\left( \frac{R}{l} \right)^n = Y^\gamma + \left( \frac{R_0}{a} \right)^n Y^{n\beta} \leq 2Y^\gamma,
\]

provided

\[
Y \leq \left( \frac{a}{R_0} \right)^{n/(n\beta - \gamma)}.
\]

Thus we have

\[
\frac{E_0(N, L)}{N} \geq s_n a^{n-2} \rho (1 - Y^\alpha) (1 - C_1 Y^{\gamma/n}) (1 - Y^{n\beta - 1}) (1 - C_2 Y^{1+\gamma-n\beta}) \times \left( 1 - \frac{C_3 Y^{1-a-2\beta-\gamma}}{1 - C_4 Y^{2-a-(n+2)\beta}} \right).
\]

In attempt to fit exponents we choose $\beta$ and $\gamma$ such that

\[
\gamma/n = \alpha = n\beta - 1,
\]

which in particular implies that $1 + \gamma - n\beta = 2\alpha$. Now, the optimal choice of $\alpha$, such that

\[
1 - \alpha - 2\beta - \gamma \geq \alpha \quad \text{and} \quad 2 - \alpha - (n + 2)\beta > 0,
\]

is given in (2.9). With this choice the requirements of Lemma 2.9 are indeed satisfied if $Y$ is sufficiently small (depending only on the dimension) and if we take $L = kl$, for an integer $k \in \mathbb{N}$. Also (2.25) is exactly the latter condition in (2.10). By letting $k \to \infty$ we therefore conclude the proof.

Corollary 2.10. Suppose that $V$ is nonnegative, radial and measurable with a decay $V(r) \leq Cr^{-\nu}$, for large $r$, where $\nu > (6n - 2)/5$. Suppose furthermore that $V$ admits a scattering solution. There exist a constant $C > 0$ depending only on $n$ and a $\delta > 0$ depending on $n, V$ such that

\[
e_0(\rho) \geq s_n a^{n-2} \rho (1 - CY^\alpha),
\]

provided $Y \leq \delta$. 

Proof. Let \( R > 0 \) and define \( V_R = V \chi_{B(0,R)} \) with scattering length \( a_R \leq a \). Since \( V \) is nonnegative, replacing \( V \) with \( V_R \) cannot increase the energy. By Theorem 2.3 we then have

\[
e_0(\rho) \geq s_n a_R^{n-2} \rho (1 - CY_R^2) \geq s_n a_R^{n-2} \rho (1 - CY^\alpha),
\]

provided \( Y_R := a_R^\alpha \rho \) is sufficiently small and

\[
Y_R \leq \left( \frac{a_R}{R} \right)^{n-2}.
\]

(2.26)

Denote the scattering solutions of \( V \) and \( V_R \) by \( u \) respectively \( u_R \). Then, by (2.6),

\[
a_R^{n-2} - a_R^{n-2} = \frac{1}{2s_n} \int V(x)u(x) - V_R(x)u_R(x) \, dx \leq \frac{1}{2s_n} \int V(x) - V_R(x) \, dx = \frac{1}{2s_n} \int_{|x| \geq R} V(x) \, dx,
\]

where the inequality follows from the fact that \( u \leq u_R \leq 1 \). From the decay of \( V \) we obtain

\[
a_R^{n-2} \geq a^{n-2} \left( 1 - \frac{K}{2(n-2)a^{n-2}R^\alpha} \right),
\]

provided \( R \) is sufficiently large. By choosing \( R \) such that

\[
\frac{K}{2(n-2)a^{n-2}R^\alpha} = Y^\alpha,
\]

it follows that \( R \) is large,

\[
a_R^{n-2} \geq a^{n-2}(1 - Y^\alpha),
\]

and (2.26) is satisfied, if \( Y \) is sufficiently small and \( \nu > (6n - 2)/5 \).

\[ \square \]

3 A Second Order Upper Bound

In this section we derive a second order upper bound to \( e_0(\rho) \) by estimating the energy in the state (1.3). The calculation is inspired by [4].

**Theorem 3.1.** Let \( n \geq 3 \) and suppose that \( V \in C_0^\infty(\mathbb{R}^n) \) is nonnegative and radially symmetric with \( V(0) > 0 \). Then

\[
e_0(\rho) \leq 4\pi a \rho \left( 1 + [1 + C\gamma] \frac{128}{15\sqrt{n}} Y^{1/2} \right) + \mathcal{O}(\rho^2 |\ln \rho|) \quad (n = 3)
\]

\[
e_0(\rho) \leq 4\pi^2 a^2 \rho \left( 1 + [1 + C\gamma]2\pi^2 Y |\ln Y| \right) + \mathcal{O}(\rho^2) \quad (n = 4)
\]

\[
e_0(\rho) \leq s_n a^{n-2} \rho + \mathcal{O}(\rho^2) \quad (n \geq 5),
\]

where

\[
\gamma := \int_{\mathbb{R}^n} V(x)|x|^{2-n} \, dx
\]

(3.1)

and \( C > 0 \) is independent of \( V \).
The assumptions on $V$ in Theorem 3.1 are presumably not optimal. In the actual grandcanonical calculation below, we only need $V$ and its Fourier transform to decay sufficiently fast at infinity (depending on the dimension), and of course the latter can be met by imposing finite smoothness on $V$. We use compact support of $V$ and $V(0) > 0$ in Lemma 3.2 below, which allows us to relate the canonical- and 'grand canonical' ground state energies. Presumably the assumption of compact support can be relaxed to a sufficiently fast decay.

In order to prove Theorem 3.1 we initially consider (1.1) with Dirichlet boundary conditions. Our calculation below is carried out in the grand canonical ensemble, and hence we consider the second quantization of $H_{NL}$

\[ H_L := \bigoplus_{N=0}^{\infty} H_{N,L} \text{ on } \mathcal{F}_L := \bigoplus_{N=0}^{\infty} L^2_{\text{sym}}(\Lambda_N^L), \tag{3.2} \]

with the corresponding 'grand canonical ground state energy'

\[ E_0^{GC}(N,L) := \inf \{ \langle H_L \rangle : \| \Psi \|_{\mathcal{F}} = 1, \langle N \rangle \Psi \geq N \}, \tag{3.3} \]

where $N = N_L$ denotes the number operator on $\mathcal{F}_L$ and $\langle A \rangle_{\Psi}$ denotes the expectation $\langle \Psi, A \Psi \rangle$ of any operator $A$ with $\Psi$ in its domain. Consider the canonical and grand canonical ground state energy per volume,

\[ e_L(\rho) := \frac{E_0(\rho L^n, L)}{L^n}, \quad e^{GC}_L(\rho) := \frac{E_0^{GC}(\rho L^n, L)}{L^n}. \tag{3.4} \]

We will assume that the limit

\[ e(\rho) := \lim_{L \to \infty} e_L(\rho) \tag{3.5} \]

is a convex function of $\rho$ (see e.g. [17]). The following result, which we prove in appendix A, shows that, in the thermodynamic limit, the canonical and grand canonical energies agree.

**Lemma 3.2.** Suppose that $V \in L^1(\mathbb{R}^n)$ is nonnegative, radially symmetric and compactly supported. Suppose furthermore that $V \geq \varepsilon \chi_{B(0,R)}$, for some $\varepsilon, R > 0$. Then

\[ e(\rho) = \lim_{L \to \infty} e^{GC}_L(\rho). \]

By (3.3) it is clear that $\rho \mapsto e^{GC}_L(\rho)$ is increasing, for any fixed $L$. As a consequence we have the following slightly stronger result.

**Corollary 3.3.** Suppose that $V$ satisfies the assumptions of Lemma 3.2 and suppose that $\rho_L \to \rho$ as $L \to \infty$. Then

\[ e(\rho) = \lim_{L \to \infty} e^{GC}_L(\rho_L) \]

**Proof.** Fix an arbitrary $\varepsilon > 0$. By assumption $e(\rho)$ is convex and hence continuous. Thus we can choose $\delta > 0$ such that

\[ |e(\rho) - e(\rho')| \leq \varepsilon, \]
A Second Order Upper Bound

for each $\rho' > 0$ with $|\rho - \rho'| \leq \delta$. Then, for $L$ sufficiently large,

$$e^{GC}_L(\rho_L) \geq e^{GC}_L(\rho - \delta)$$

$$= [e^{GC}_L(\rho - \delta) - e(\rho - \delta)] + e(\rho - \delta)$$

$$\geq [e^{GC}_L(\rho - \delta) - e(\rho - \delta)] + e(\rho) - \varepsilon.$$

By Lemma 3.2 it then follows that

$$\liminf_{L \to \infty} e^{GC}_L(\rho_L) \geq e(\rho) - \varepsilon.$$

Similarly we can show a consistent upper bound, and since $\varepsilon$ was arbitrary, the result follows.

In Section 3.1 we construct a periodic trial state with an expected number of particles $\langle N \rangle = \rho L^n$, not directly leading to an upper bound on $e_0(\rho)$ via Lemma 3.2. However, Lemma 3.4 below, which is essentially proved in [22], shows that given any periodic state, we can find a Dirichlet state on a slightly larger box, with almost as low energy. We let

$$V_L(x) := \sum_{m \in \mathbb{Z}^n} V(x + mL) = \frac{1}{L^n} \sum_{p \in \Lambda^*_L} \hat{V}_p e^{ip \cdot x}, \quad x \in \mathbb{R}^n$$

denote the $L$-periodization of $V$, where $\Lambda^*_L := (2\pi/L)\mathbb{Z}^n$ and

$$\hat{V}_p := \int_{\mathbb{R}^n} e^{-ip \cdot x} V(x) dx$$

denotes the Fourier transform of $V$, which is real-valued and radially symmetric, since $V$ is. Then let

$$\tilde{H}_{N,L} := \sum_{i=1}^N -\Delta_i + \sum_{1 \leq j < k \leq N} V_L(x_j - x_k)$$

with periodic boundary conditions, and let $\tilde{H}_L$ denote its second quantization. Note that, since $V$ is nonnegative, it is clear that $V \leq V_L$, and hence the transition from $V$ to $V_L$ cannot decrease the energy. However, since $V_L \to V$ pointwise as $L \to \infty$, we expect the ground state energy of the two systems to coincide in the thermodynamic limit.

Lemma 3.4. Let $L > 2l > 0$. Then

$$E^{GC}_0(N, L + 2l) \leq \langle \tilde{H}_L \rangle_\Psi + CN^N/L,$$

for each periodic, normalized $\Psi \in \mathcal{F}_L$ with $\langle N \rangle_\Psi = N$. Here $C > 0$ depends only on $n$.

We apply Lemma 3.4 with $l := \sqrt{L}/2$ and notice that

$$\frac{E^{GC}_0(\rho L^n, L + 2l)}{\rho L^n} = \frac{E^{GC}_0(\rho L + 2l, (L + 2l)^n, L + 2l)}{\rho L + 2l (L + 2l)^n},$$

where

$$\rho_L := \frac{\rho(L - 2l)^n}{L^n} \to \rho \quad \text{as} \quad L \to \infty.$$
Together with Corollary 3.3 we conclude that

$$c_0(\rho) \leq \limsup_{L \to \infty} \frac{\langle \tilde{H}_L \rangle_{\Psi}}{\rho L^n},$$

for each periodic, normalized $\Psi \in \mathcal{F}_L$ with expected number of particles $\langle N \rangle_{\Psi} = \rho L^n$.

Finally, we note that, with the periodic potential $V_L$, we have (in the sense of quadratic forms)

$$\tilde{H}_L = \sum_p p^2 a_p^+ a_p + \frac{1}{2L^n} \sum_{p \neq q, r, s} \hat{V}_{p-r} a_p^+ a_q^+ a_r a_s,$$

(3.6)

where all sums are over $\Lambda_L^*$ and where $a_p^+$ and $a_p$ denote the bosonic creation and annihilation operators on $\mathcal{F}_L$ w.r.t. the plane wave $x \mapsto L^{-n/2} e^{ip \cdot x}$.

3.1 The Trial State

The state in (1.3) can be defined as follows. Fix $\rho, L > 0$ and set $N := \rho |\Lambda| = \rho L^n$. Then let

$$\Psi := \sum_{\alpha} f(\alpha) |\alpha\rangle$$

(3.7)

where $\{ |\alpha\rangle \}_\alpha \subset \mathcal{F}$ is the orthonormal basis given by

$$|\alpha\rangle := \prod_{k \in \Lambda^*} \frac{1}{\sqrt{\alpha(k)!}} (a_k^+) \alpha(k) |0\rangle,$$

for each $\alpha : \Lambda^* \to \mathbb{N}_0$ with $|\alpha| := \sum_{k \in \Lambda^*} \alpha(k) < \infty$. Note that, by the canonical commutation relations,

$$a_p |\alpha\rangle = \sqrt{\alpha(p)} (|\alpha - \delta_p\rangle)$$

and

$$a_p^+ |\alpha\rangle = \sqrt{\alpha(p) + 1} |\alpha + \delta_p\rangle,$$

(3.8)

for any $p \in \Lambda^*$, where $\delta_p(k) := \delta_{p,k}$. Let

$$\mathcal{M} := \{ \alpha : \Lambda^* \to \mathbb{N}_0 : |\alpha| < \infty \text{ and } \alpha(-p) = \alpha(p) \text{ for each } p \in \Lambda^* \},$$

We define the coefficient function $f$ in (3.7) by

$$f(\alpha) := \exp \left( N_0 + \sum_{p \neq 0} |\ln(1 - c_p^2)| \right)^{-1/2} \cdot \left( \frac{N_0^\alpha(0)}{\alpha(0)!} \prod_{p \neq 0} c_p^\alpha(p) \right)^{1/2},$$

(3.9)

for $\alpha \in \mathcal{M}$ and $f(\alpha) = 0$ otherwise. Here $c : \Lambda^* \setminus \{0\} \to (-1, 1)$ is to be chosen and

$$N_0 := N - \sum_{p \neq 0} c_p^2 \frac{c_p^2}{1 - c_p^2}.$$

(3.10)

It will be apparent later on that (3.10) is equivalent to the condition $\langle \Psi, \mathcal{N} \Psi \rangle = N$. We will assume that $c_{-p} = c_p$, for each $p$ and clearly we also need some decay of $c_p$ in order for the sums in (3.9) and (3.10) to converge. Given any operator $A$ with a domain
containing $\Psi$, we let $\langle A \rangle := \langle \Psi, A\Psi \rangle$ denote the expectation of $A$ in the state $\Psi$. Most of the interaction terms in (3.6) have zero expectation in the state $\Psi$. In fact, since $f$ vanishes outside $\mathcal{M}$ and since $\alpha(-p) = \alpha(p)$, for each $p \in \Lambda^*$ and each $\alpha \in \mathcal{M}$, it follows that only pair interactions terms where either $p = r$, $p = s$ or $p = -q$ have nonzero expectation in $\Psi$. Thus

$$\langle \hat{H}_L \rangle = \sum_p p^2 \langle a_p^+ a_p \rangle + E_1 + E_2 + E_3,$$

where

$$E_1 := \frac{V_0}{2|\Lambda|} \sum_{p,q} \langle a_p^+ a_q^+ a_p a_q \rangle, \quad E_2 := \frac{1}{2|\Lambda|} \sum_{p \neq q} \hat{V}_{p-q} \langle a_p^+ a_q^+ a_p a_q \rangle$$

and

$$E_3 := \frac{1}{2|\Lambda|} \sum_{p \neq \pm q} \hat{V}_{p-q} \langle a_p^+ a^- a_q a^- \rangle.$$

Lemma 3.5 below provides us with all the relevant expectations in terms of $N_0$ and $c_p$.

We introduce the notation

$$h_p := \frac{c_p^2}{1 - c_p^2} \quad \text{and} \quad s_p := \frac{c_p}{1 - c_p}.$$

**Lemma 3.5.** Let $p, q \in \Lambda^*$ with $p \neq \pm q$ and $p \neq 0$. Then

1. $\langle a_0^+ a_0 \rangle = N_0 = \langle a_0 a_0 \rangle$ and $\langle a_0^+ a_0 a_q a_0 \rangle = N_0(N_0 + 1)$
2. $\langle a_p^+ a_p a_q^+ a_q \rangle = \langle a_p^+ a_p \rangle \cdot \langle a_q^+ a_q \rangle$
3. $\langle a_p^+ a_{-p}^+ a_q^+ a_q \rangle = \langle a_p^+ a_{-p}^+ \rangle \cdot \langle a_q a_q \rangle$
4. $\langle a_p^+ a_p \rangle = h_p$
5. $\langle a_p^+ a_{-p}^+ \rangle = s_p$
6. $\langle a_p^+ a_p a_{-p}^+ a_{-p} \rangle = h_p(2h_p + 1)$

**Proof.** The identities are proved similarly, so we only show a few of them. By definition of $\Psi$ and the relations (3.6), we have

$$\langle a_p^+ a_p \rangle = \sum_{\alpha} \alpha(p)|f(\alpha)|^2,$$

for any $p \in \Lambda^*$. Define the operation $A^0\alpha := \alpha + \delta_0$ and $A^p\alpha := \alpha + \delta_p + \delta_{-p}$, for $p \neq 0$. Notice that

$$f(A^0\alpha) = N_0^{1/2}(\alpha(0) + 1)^{-1/2}f(\alpha) \quad \text{and} \quad f(A^p\alpha) = c_p f(\alpha).$$

We then have

$$\langle a_0^+ a_0 \rangle = \sum_{\alpha \in A^0(\mathcal{M})} \alpha(0)|f(\alpha)|^2 = \sum_{\beta} (\beta(0) + 1)|f(A^0\beta)|^2 = N_0.$$
where we have also used that $\sum_\beta |f(\beta)|^2 = 1$ due to normalization. For $p \neq 0$ we get

$$\langle a_p^+ a_p \rangle = \sum_\beta (\beta(p) + 1) |f(A^p \beta)|^2 = c_p^2 ((a_p^+ a_p) + 1),$$

and solving for $\langle a_p^+ a_p \rangle$ yields 4. Also,

$$\langle a_p^+ a_p^+ \rangle = \sum_\alpha f(A^p \alpha)f(\alpha) (\alpha(p) + 1) = c_p (h_p + 1) = s_p,$$

as claimed.

Notice that, by Lemma 3.5,

$$\langle \mathcal{N} \rangle = \sum_p \langle a_p^+ a_p \rangle = N_0 + \sum_{p \neq 0} h_p,$$

and hence the condition $\langle \mathcal{N} \rangle = N$ is indeed equivalent to (3.10).

### 3.2 Computation of the Energy

Eventually we will choose $c_p$ via the new variable $e_p := \frac{c_p}{1 + c_p}$, $h_p = \frac{c_p^2}{1 - 2c_p}$, $s_p = \frac{e_p(1 - e_p)}{1 - 2e_p}$.

Note that the constraint $|c_p| < 1$ is equivalent to $e_p < 1/2$. In Lemma 3.6 below we calculate the energy $\langle \tilde{H}_L \rangle$ per particle in the thermodynamic limit

$$E(\rho) := \lim_{L \to \infty} \frac{\langle \tilde{H}_L \rangle}{\rho L^n}.$$  

For this reason, it is convenient to assume that $e_p$ is independent of $L$, i.e. we assume that $c$ is defined on $\mathbb{R}^n \setminus \{0\}$ rather than on $\Lambda^* \setminus \{0\}$. We will also employ the fact that for any continuous function $F \in L^1(\mathbb{R}^n)$, decaying faster than $|p|^{-n-\varepsilon}$ at infinity, for some $\varepsilon > 0$, we have the convergence

$$\lim_{L \to \infty} \frac{1}{L^n} \sum_{p \in \Lambda^*} F(p) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} F(p) \, dp. \quad (3.11)$$

We denote the scattering solution by $1 - w$ and set

$$\varphi := Vw \quad \text{and} \quad g := V - \varphi = V(1 - w).$$

Note that $\hat{g}_0 = 2s_n a_n^{n-2}$ by (2.6). Though $w$ is not integrable, it follows from the scattering equation (2.2) that, as tempered distribution, $\hat{w}$ equals the function $p \mapsto \hat{g}_p/(2p^2)$. We shall abuse notation slightly by denoting

$$\hat{w}_p := \frac{\hat{g}_p}{2p^2}.$$
Lemma 3.6. Suppose that \( e : \mathbb{R}^n \setminus \{0\} \to (-\infty, 1/2) \) is even, continuous and integrable with fast decay. Then

\[
E(\rho) = s_n a^{n-2}\rho + Q + \Omega,
\]

where

\[
Q := \frac{1}{2(2\pi)^n \rho} \int p^2 \left[ \frac{e_p^2}{1 - 2e_p} + (\rho \tilde{w}_p)^2 \right] dp,
\]

\[
\tilde{Q} := \frac{2}{(2\pi)^n} \int \hat{\varphi}_p \rho p dp,
\]

\[
\Omega := \frac{1}{2(2\pi)^n \rho} \int \int [\hat{V}_{p-q}(e_p + \rho \tilde{w}_p)(e_q + \rho \tilde{w}_q) + 2(\hat{V}_{p-q} - \hat{V}_p)s_p h_q - 2\hat{V}_p h_p h_q] dp dq.
\]

Proof. By Lemma 3.5, the kinetic energy is simply

\[
\sum_p p^2 \langle a_p a_p^+ \rangle = \sum_{p \neq 0} p^2 h_p = \sum_{p \neq 0} \frac{p^2 e_p^2}{1 - 2e_p}.
\]

Using commutation relations, Lemma 3.5 and (3.10), we find that

\[
E_1 = \frac{\hat{V}_0}{2|\Lambda|} \left( \sum_{p, q} \langle a_p^+ a_p a_q^+ a_q \rangle - \sum_p \langle a_p^+ a_p \rangle \right) = \frac{\hat{V}_0}{2|\Lambda|} \left( N^2 + \sum_{p \neq 0} h_p (h_p + 1) \right),
\]

where the last sum comes from the special cases \( p = \pm q \). Note that contributions like that will vanish in the energy per particle in the thermodynamic limit. Similarly,

\[
E_2 = \frac{N_0}{|\Lambda|} \sum_{p \neq 0} \hat{V}_p h_p + \frac{1}{2|\Lambda|} \sum_{p \neq 0} \hat{V}_{2p} h_p (2h_p + 1) + \frac{1}{2|\Lambda|} \sum_{p \neq 0} \hat{V}_{p-q} h_p h_q
\]

\[
= \sum_{p \neq 0} \rho \hat{V}_p h_p - \frac{1}{|\Lambda|} \sum_{p, q \neq 0} \hat{V}_p h_p h_q + \frac{1}{2|\Lambda|} \sum_{p \neq 0} \hat{V}_{2p} h_p (2h_p + 1) + \frac{1}{2|\Lambda|} \sum_{p, q \neq 0} \hat{V}_{p-q} h_p h_q,
\]

and also

\[
E_3 = \sum_{p \neq 0} \rho \hat{V}_p s_p - \frac{1}{|\Lambda|} \sum_{p, q \neq 0} \hat{V}_p s_p h_q + \frac{1}{2|\Lambda|} \sum_{p, q \neq 0} \hat{V}_{p-q} s_p s_q.
\]

Thus, in the limit \( L \to \infty \),

\[
E(\rho) = \frac{\hat{V}_0 \rho}{2} + \frac{1}{(2\pi)^n \rho} \int p^2 e_p^2 + \rho \hat{V}_p e_p dp + \frac{1}{2(2\pi)^n \rho} \int \int \hat{V}_{p-q} s_p s_q - 2\hat{V}_p s_p h_q dp dq + \frac{1}{2(2\pi)^n \rho} \int \int \hat{V}_{p-q} h_p h_q - 2\hat{V}_p h_p h_q dp dq.
\]

By the relation \( e_p = s_p - h_p \) we have

\[
\int \int \hat{V}_{p-q} s_p s_q - 2\hat{V}_p s_p h_q dp dq = \int \int \hat{V}_{p-q} (e_p e_q - h_p h_q) + 2(\hat{V}_{p-q} - \hat{V}_p) s_p h_q dp dq.
\]

\[20\]


and hence

\[ E(\rho) = \frac{\hat{V}_0\rho}{2} + \frac{1}{(2\pi)^n \rho} \int \frac{p^2 e_p^2 + \rho \hat{V}_p e_p}{1 - 2e_p} \, dp + \frac{1}{2(2\pi)^{2n} \rho} \int \hat{V}_{p-q} e_p e_q \, dp \, dq \]

\[ + \frac{1}{(2\pi)^{2n} \rho} \int \int (\hat{V}_{p-q} - \hat{V}_p) s_p h_q - \hat{V}_p h_p h_q \, dp \, dq. \]

Now, using \((2\pi)^n \hat{\varphi} = \hat{V} \ast \hat{\varphi}\), and \(V = g + \varphi\), we get

\[ \frac{\hat{V}_0\rho}{2} + \frac{\rho}{2(2\pi)^n} \int \hat{V}_p \hat{\varphi}_p \, dp = \frac{s_n a_n - 2}{\rho} \int \frac{\hat{g}_p \hat{\varphi}_p \, dp}{2(2\pi)^n} + \frac{\rho}{2(2\pi)^n} \int \hat{\varphi}_p \hat{\varphi}_p \, dp \]

and also

\[ \frac{1}{2(2\pi)^{2n} \rho} \int \int \hat{V}_{p-q} e_p e_q \, dp \, dq = \frac{1}{2(2\pi)^{2n} \rho} \int \int \hat{V}_{p-q} (e_p + \rho \hat{\varphi}_p)(e_q + \rho \hat{\varphi}_q) \, dp \, dq \]

\[ - \frac{1}{(2\pi)^n} \int \hat{\varphi}_p \hat{\varphi}_p \, dp - \frac{\rho}{2(2\pi)^n} \int \hat{\varphi}_p \hat{\varphi}_p \, dp. \]

Combining terms yields the desired. \(\Box\)

In [1] the function \(e_p\) is chosen as the pointwise minimizer of the sum of integrands in \(Q\) and \(\hat{Q}\). However, it turns out that including the latter in the minimization problem does not lower the energy significantly. In fact, the calculation of Yau-Yin [22] suggests that \(\hat{Q}\) is really not present in the ground state energy, but should rather be cancelled by a term 'missing' in the energy of our trial state. Thus we will choose \(e_p\) to minimize the simpler expression

\[ m_p := \frac{e_p^2 + 2\rho \hat{\varphi}_p e_p}{1 - 2e_p}. \]

This yields

\[ -e_p^2 + e_p + \rho \hat{\varphi}_p = 0, \quad e_p = \frac{1}{2} \left( 1 - \sqrt{1 + 4\rho \hat{\varphi}_p} \right) \quad (3.12) \]

and

\[ m_p = \frac{(1 - 2e_p)(-e_p - \rho \hat{\varphi}_p) + (-e_p^2 + e_p + \rho \hat{\varphi}_p)}{1 - 2e_p} = \frac{1}{2} \left( \sqrt{1 + 4\rho \hat{\varphi}_p} - 1 - 2\rho \hat{\varphi}_p \right), \]

provided \(1 + 4\rho \hat{\varphi}_p \geq 0\). Note however that, since \(\hat{g}\) is continuous, \(\hat{g}_0 > 0\) and \(\hat{g}_p \rightarrow 0\) as \(|p| \rightarrow \infty\), it follows that \(\hat{\varphi}_p\) is bounded from below; and hence

\[ \lim \inf_{\rho \rightarrow 0} \left[ \inf_{p \neq 0} (1 + 4\rho \hat{\varphi}_p) \right] \geq 1. \]

With the choice in (3.12) we have

\[ Q = \frac{1}{2(2\pi)^n \rho} \int p^2 \Phi(\rho \hat{\varphi}_p) \, dp, \quad (3.13) \]

where

\[ \Phi(t) := \sqrt{1 + 4t} + 2t^2 - 2t - 1. \quad (3.14) \]

Finally, we note that \(|e_p| \leq \rho |\hat{\varphi}_p|\), for \(|p| \gg \rho^{1/2}\), and hence \(e\) inherits decay from \(\hat{g}\).
3.3 Estimates

In this section we estimate the integrals from Lemma 3.6 in the limit $\rho \to 0$, given the particular choice in (3.12). We begin with the term $Q$, and in fact we will derive asymptotics of order up to $\sim n/2$ with coefficients, all except one, given in terms of integrals of $\hat{w}_p$ (see also Table 1 below). We stress, however, that the physical relevance of these higher order asymptotics remains to be understood. In fact, while the main contribution in dimension three and four comes from $Q$, we believe that $\Omega$ and $Q$ are of the same leading order in dimension $n \geq 5$.

Lemma 3.7. In dimension $n = 3$, 

$$Q = (4\pi a \rho) \cdot \frac{128}{15\sqrt{\pi}} \, Y^{1/2} + o(\rho^{3/2}) \quad \text{and} \quad Q \leq (4\pi a \rho) \cdot \frac{128}{15\sqrt{\pi}} \, Y^{1/2}. \quad (3.16)$$

In dimension $n \geq 4$, 

$$Q = \sum_{m=3}^{[n/2]} c_m \rho^{n-1} + c_{n/2+1} \left( s_n a^{n-2} \rho Y^{n/2-1} |\ln Y| \right) + O(\rho^{n/2}),$$

where the error term depends on $V$ and where $c_m = 0$ if $m \notin \mathbb{N}$,

$$c_m := \frac{\Phi^{(m)}(0)}{2(2\pi)^n m!} \int_{\mathbb{R}^n} p^2 \hat{w}_p^m, \quad m \leq (n+1)/2,$$

and

$$c_{n/2+1} := \frac{\Phi^{(n/2+1)}(0)|s_n a^{n-1}| / 2(n/2+1)!}{4(2\pi)^n (n/2+1)!}.$$

The function $\Phi$ is given in (3.14).

Proof. We first consider the case $n = 3$. Let $\varepsilon = (\hat{g}_0 \rho)^{1/2}$. By a change of variables $p \mapsto \varepsilon p$, continuity of $\hat{g}$ and the dominated convergence theorem we have

$$\rho^{-3/2} Q = \frac{\hat{g}_0^{5/2}}{2(2\pi)^3} \int_{\mathbb{R}^3} p^2 \Phi \left( \frac{\varepsilon p}{2p^2 \hat{g}_0} \right) dp \to \frac{\hat{g}_0^{5/2}}{2(2\pi)^3} \int_{\mathbb{R}^3} p^2 \Phi \left( \frac{1}{2p^2} \right) dp \quad (3.15)$$

as $\rho \to 0$. A direct calculation then yields

$$Q = (4\pi a \rho) \cdot \frac{128}{15\sqrt{\pi}} \, Y^{1/2} + o(\rho^{3/2}). \quad (3.16)$$

The explicit upper bound claimed in the lemma can be obtained from the same calculation with the additional information that $\Phi$ is increasing and $\hat{g}_p \leq \hat{g}_0$. In [4] the estimate is done more carefully and shows that (3.16) holds with $o(\rho^{3/2})$ replaced by $O(\rho^2 |\ln \rho|)$. In higher dimensions the asymptotics of $Q$ is more subtle, due to the fact that the latter integral in (3.15) becomes divergent! That is, we cannot replace $\hat{g}_p$ by $\hat{g}_0$, because we
need the decay of \( \hat{g} \) in order for the integral to converge. However, from the asymptotics of \( \Phi \) we get some information. First notice that \( \Phi(0) = \Phi'(0) = \Phi''(0) = 0 \), we have

\[
Q'_{\varepsilon} := \frac{1}{2(2\pi)^n \rho} \int_{|p| \leq \varepsilon} p^2 \Phi(p \hat{\omega}_p) \, dp \leq \frac{1}{2(2\pi)^n \rho} \int_{|p| \leq \varepsilon} p^2 2(p \hat{\omega}_p)^2 \, dp \\
\leq \frac{\hat{g}_0 \rho}{4(2\pi)^n} \int_{|p| \leq \varepsilon} p^{-2} \, dp = C a^{n-2} \rho Y^{n/2-1},
\]

where we have inserted \( \hat{g}_0 = 2s_n a^{n-2} \). To estimate \( Q_{\varepsilon} := Q - Q'_{\varepsilon} \), we expand \( \Phi \) to the \((k-1)\) th order around \( t = 0 \), where \( k \) is the smallest integer such that \( 2k \geq n + 3 \). Since \( \Phi(0) = \Phi'(0) = \Phi''(0) = 0 \), we have

\[
\Phi(t) = b_3 t^3 + \ldots + b_{k-1} t^{k-1} + O(t^k),
\]

where \( b_m := \Phi^{(m)}(0)/m! \). Correspondingly we have the expansion

\[
Q_{\varepsilon} = Q_{\varepsilon}^{(3)} + \ldots + Q_{\varepsilon}^{(k-1)} + \mathcal{E},
\]

where

\[
Q_{\varepsilon}^{(m)} := \frac{b_m}{2(2\pi)^n \rho} \int_{|p| \geq \varepsilon} p^2 (p \hat{\omega}_p)^m \, dp.
\]

and where

\[
|\mathcal{E}| \leq C \rho^{-1} \int_{|p| \geq \varepsilon} |p \hat{\omega}_p|^k \, dp \leq C \hat{g}_0^k \rho^{-1} \int_{|p| \geq \varepsilon} p^{2-2k} \, dp = C a^{n-2} \rho Y^{n/2-1}.
\]

If \( m < n/2 + 1 \), then \( p^2 \hat{\omega}_p^m \) is integrable at \( p = 0 \), and we have

\[
Q_{\varepsilon}^{(m)} = \frac{b_m \rho^m}{2(2\pi)^n} \int_{|p| \geq \varepsilon} p^2 \hat{\omega}_p^m \, dp + O(a^{n-2} \rho Y^{n/2-1}).
\]

Notice that if \( n \) is odd, then \( k = (n + 3)/2 \), and hence \( m < n/2 + 1 \), for each \( m \leq k - 1 \). In equal dimension there is a \( m = n/2 + 1 \) term:

\[
Q_{\varepsilon}^{(m)} = \frac{b_m}{2(2\pi)^n \rho} \int_{|p| \leq 1} p^2 (p \hat{\omega}_p)^m \, dp + O(\rho^{m-1})
\]

\[
= \frac{b_m}{2(2\pi)^n \rho} \int_{|p| \leq 1} p^2 \left( \frac{\hat{g}_0}{2p^2} \right)^m \, dp + O(\rho^{m-1}),
\]

where the errors depend on \( V \), and where we have used Lipschitz continuity of \( \hat{g} \) to replace \( \hat{g}_p \) with \( \hat{g}_0 \) in the second estimate. Now, by inserting \( \hat{g}_0 = 2s_n a^{n-2} \), we get

\[
Q_{\varepsilon}^{3/2+1} = s_n a^{n-2} \rho \frac{b_{n/2+1} \rho^{n-1} |\ln Y| \rho^{n/2} + O(\rho^{n/2})}{4(2\pi)^n} Y^{n/2-1} |\ln Y| + O(\rho^{n/2}),
\]

where we have artificially replaced \( |\ln(\hat{g}_0\rho)| \) by \( |\ln Y| \) at the cost of an error of order \( \rho^{n/2} \), depending on \( V \). In particular, with \( b_3 = 4 \) and \( |S^3| = 2\pi^2 \), we have

\[
Q_{2}^{(3)} = (4\pi^2 a^2 \rho) \cdot 2\pi^2 Y |\ln Y| + O(\rho^2),
\]

which is the term present in four dimensions.
### A Second Order Upper Bound

| $n$ | $Q$                     |
|-----|-------------------------|
| 3   | $\rho^{3/2} \cdot O(\rho^2 |\ln \rho|)$ |
| 4   | $\rho^2 |\ln \rho| \cdot O(\rho^2)$ |
| 5   | $\rho^2 \cdot O(\rho^{5/2})$ |
| 6   | $\rho^2 \cdot \rho^3 |\ln \rho| \cdot O(\rho^3)$ |
| 7   | $\rho^2 \cdot \rho^3 \cdot O(\rho^{7/2})$ |
| :  | :                      |

Table 1: Qualitative expansion of $Q$ in the first few dimensions.

In table 1 we have listed the powers of $\rho$ in the expansion of $Q$ up to dimension $n = 7$. Whether the expansion of $e_0(\rho)$ has this structure too remains to be clarified.

**Lemma 3.8.**

$$
\Omega(\rho) = \begin{cases} 
O(\rho^2 |\ln \rho|) & n = 3 \\
O(\rho^2) & n \geq 4 
\end{cases}
$$

**Proof.** Using $|\hat{V}_p| \leq \hat{V}_0$, Lipschitz continuity of $\hat{V}$ and the relation in (3.12), we have

$$
|\Omega| \leq C_V^{-1} \left\{ \left( \int e^2_p \, dp \right)^2 + \left( \int |s_p| \, dp \right) \left( \int h_q |q| \, dq \right) + \left( \int h_p \, dp \right)^2 \right\}.
$$

Notice the asymptotics

$$
h_p = \frac{1}{2} \left( \frac{1 + 2 \rho \hat{w}_p}{\sqrt{1 + 4 \rho \hat{w}_p}} - 1 \right) = \begin{cases} 
O(\sqrt{\rho \hat{w}_p}) & |\rho \hat{w}_p| \to \infty \\
O(\rho^2 \hat{w}_p^2) & |\rho \hat{w}_p| \to 0 
\end{cases}.
$$

In fact, $h_p \leq C \rho^2 \hat{w}_p^2$ for each $p \neq 0$, provided $\rho$ is sufficiently small. In dimension $n \geq 5$ we then simply have

$$
\int h_p \, dp = O(\rho^2 \|\hat{w}\|_2^2).
$$

Otherwise we split the integral into two parts

$$
\int h_p \, dp \leq C \left[ \int_{|p| \leq \varepsilon} (\rho \hat{w}_p)^{1/2} \, dp + \int_{|p| > \varepsilon} (\rho \hat{w}_p)^2 \, dp \right] = I_1 + I_2
$$

where $\varepsilon := (\alpha \rho)^{1/2}$. Since $\hat{g}_p \leq \hat{g}_0 = 2 s_n a^{n-2}$, it follows that $I_1 = O(\rho Y^{n/2-1})$. In dimension $n = 3$ we again use $|\hat{g}_p| \leq \hat{g}_0$ to obtain $I_2 = O(\rho Y^{1/2})$, and in four dimensions we get a logarithmic term,

$$
I_2 \leq C \rho Y |\ln Y| + C_V \rho^2.
$$

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In total,
\[
\int h_p \, dp \leq \begin{cases} 
C \rho Y^{1/2} & n = 3 \\
C \rho Y \ln Y + C_V \rho^2 & n = 4 \\
C_V \rho^2 & n \geq 5
\end{cases}.
\tag{3.17}
\]

By repeating the above estimates with an additional factor \(|p|\) in the integrands, we see that
\[
\int |p|h_p \, dp \leq \begin{cases} 
C_V \rho^2 |\ln \rho| & n = 3 \\
C_V \rho^2 & n \geq 4
\end{cases}.
\]

The integral of \(e_p^2\) is estimated similarly to \(h_p\) and in fact (3.17) holds with \(h_p\) replaced by \(e_p^2\). Finally, since
\[
s_p = \frac{-\rho \hat{w}_p}{\sqrt{1 + 4 \rho \hat{w}_p}},
\]
we see that
\[
\int |s_p| \, dp = O(\rho),
\]
for any \(n \geq 3\), and we are done. \(\Box\)

**Remark 3.9.** From the estimate (3.17) and \(|\hat{\varphi}_p| \leq \hat{\varphi}_0\) it follows that
\[
\hat{Q}(p) \leq \begin{cases} 
C \hat{\gamma} a \rho Y^{1/2} & n = 3 \\
C \hat{\gamma} a^2 \rho Y \ln \rho + C_V \rho^2 & n = 4 \\
C_V \rho^2 & n \geq 5
\end{cases},
\]

where \(\hat{\gamma} := \varphi_0/\hat{g}_0\).

In order to finish the proof of Theorem 3.1, we only need to show that \(\hat{\gamma} \leq C \gamma\) as defined in (3.1). This, however, follows easily from (2.4) and (2.6), since then
\[
\hat{\varphi}_0 = \int V(x) \varphi(x) \, dx \leq a^{n-2} \int V(x)|x|^{2-n} \, dx = \frac{\hat{g}_0}{2^{\gamma} \pi_n} \int V(x)|x|^{2-n} \, dx,
\]
as desired.

## A  Equivalence of Ensembles

In this section we prove Lemma 3.2. We will see that the canonical and grand canonical energies are related via the Legendre transform, and in order for this to be well-behaved globally, it is convenient to have high density bounds on the ground state energy. A trivial upper bound to \(E_0(N, L)\) with periodic boundary conditions is obtained by calculating the energy of the constant function:
\[
E_0(N, L) \leq \frac{N(N-1)}{2|\Lambda|} \int V(x) \, dx.
\]
Thus, in the thermodynamic limit (and for all boundary conditions),
\[ \epsilon_0(\rho) \leq \frac{\hat{V}_0}{2} \rho. \] (A.1)

In the following lemma we derive a simple lower bound to \( E_0(N, L) \) under the assumption that \( V \) is uniformly strictly positive in a neighborhood of the origin. Due to lack of space, this forces a large fraction of the particles to interact.

**Lemma A.1.** Suppose that \( V \geq \epsilon \chi_{B(0,2R)} \), for some \( \epsilon, R > 0 \). Then
\[ E_0(N, L) \geq C\epsilon R \frac{n N^2}{|\Lambda|} - \frac{N}{2} V(0), \] (A.2)
for some constant \( C > 0 \) depending only on the dimension.

**Proof.** We will simply discard the kinetic energy and show that the total interaction is pointwise bounded from below by the RHS in (A.2). Let \( \chi_R = \chi_{B(0,R)} \). By Jensen’s inequality we have
\[ \left( \int_\Lambda \sum_{j=1}^N \chi_R(x_j - z) \frac{dz}{|\Lambda|} \right)^2 \leq \frac{1}{|\Lambda|} \sum_{j,k} \int_\Lambda \chi_R(x_j - z) \chi_R(x_k - z) \, dz. \]

However, the triangle inequality shows that
\[ \chi_R(x_j - z) \chi_R(x_k - z) \leq \chi_{2R}(x_j - x_k) \chi_R(x_k - z), \]
and hence
\[ \left( \int_\Lambda \sum_{j=1}^N \chi_R(x_j - z) \frac{dz}{|\Lambda|} \right)^2 \leq \frac{v_n R^n}{|\Lambda|} \sum_{j,k} \chi_{2R}(x_j - x_k) \leq \frac{v_n R^n}{\epsilon |\Lambda|} \sum_{j,k} V(x_j - x_k) \]
\[ = \frac{v_n R^n}{\epsilon |\Lambda|} \left( 2 \sum_{j<k} V(x_j - x_k) + NV(0) \right), \]
where \( v_n \) denotes the volume of the unit ball in \( \mathbb{R}^n \). The result now follows by noting that
\[ \int_\Lambda \sum_{j=1}^N \chi_R(x_j - z) \, dz \geq N v_n 2^{-n} R^n, \]
where the inequality and the factor \( 2^{-n} \) comes from the situation where \( x_j \) is located close the corner of the box. \( \square \)

Recall the notation in (3.4) and (3.5) for the ground state energy per volume. As a technical convenience we extend, for fixed \( L > 0 \), the mapping \( N \mapsto E_0(N, L) \) to \([0, \infty)\), as a piecewise linear function, by setting \( E(0, L) = 0 \) and
\[ E_0(N + \sigma, L) = (1 - \sigma) E_0(N, L) + \sigma E_0(N + 1, L), \quad \sigma \in [0, 1]. \] (A.3)
Note that, as a consequence of Lemma A.1 we have the lower bounds
\[ e_L(\rho) \geq C_1\rho^2 - C_2\rho \quad \text{and} \quad e(\rho) \geq C_1\rho^2 - C_2\rho, \]  
for constants \( C_1, C_2 > 0 \) depending on \( V \).

Since each \( N \)-particle sector is naturally imbedded in the Fock space, it follows that \( E_{0 \text{GC}}(N, L) \leq E_0(N, L) \). We remark that in case \( N \) is not a natural number, the inequality follows from the convention (A.3) by considering the combination
\[ \Psi := \sqrt{1 - \sigma} \Psi_{\lfloor N \rfloor} + \sqrt{\sigma} \Psi_{\lceil N \rceil} \]
of arbitrary \( \lfloor N \rfloor \)-particle and \( \lceil N \rceil \)-particles states, where \( \sigma := N - \lfloor N \rfloor \). In order to prove Lemma 3.2, we therefore only need to show that
\[ \liminf_{L \to \infty} e_{0 \text{GC}}^L(\rho) \geq e(\rho). \]  
We introduce a chemical potential \( \mu \geq 0 \) and notice that, for any normalized \( \Psi = (\Psi_0, \Psi_1, \ldots) \in \mathcal{F} \) with \( \langle \Psi, N \Psi \rangle \geq \rho L_n \) we have the lower bound
\[ \frac{\langle \Psi, H_L \Psi \rangle}{L^n} = \frac{1}{L^n} \left[ \mu \langle \Psi, N \Psi \rangle + \langle \Psi, (H_L - \mu N) \Psi \rangle \right] \]
\[ \geq \mu \rho + \sum_{N=0}^{\infty} \| \Psi_N \|^2 \left[ e_L(N/L^n) - \mu \frac{N}{L^n} \right] \]
\[ \geq \mu \rho + \rho \rho, \]
where \( f_L := -e_L^* \) and where
\[ g^*(\mu) := \sup_{\rho \geq 0} [\mu \rho - g(\rho)], \]
denotes the Legendre Transform of any function \( g : [0, \infty) \to \mathbb{R} \), and for \( \mu \geq 0 \) such that the supremum is finite. We will employ the well-known fact [19] that the Legendre transform is involute on convex functions, meaning that \( (g^*)^* = g^* \). The inequality (A.5) will then follow, provided we can show the convergence
\[ \lim_{L \to \infty} f_L(\mu) = f(\mu) := -e^*(\mu), \]
for each \( \mu \geq 0 \). Now, by definition,
\[ f_L(\mu) \leq e(\rho) - \mu \rho + [e_L(\rho) - e(\rho)], \]
and hence
\[ \limsup_{L \to \infty} f_L(\mu) \leq e(\rho) - \mu \rho, \]
for each \( \rho \geq 0 \). It follows that
\[ \limsup_{L \to \infty} f_L(\mu) \leq f(\mu). \]

For the lower bound we employ the following lemma.
Lemma A.2. Suppose that $V$ is compactly supported with, say, $\text{supp}(V) \subset B(0, R)$. Then

$$e_L(\rho) \geq (1 + R/L)^n e(\rho[1 + R/L]^{-n})$$

for each $\rho, L > 0$.

Proof. By convexity of $e(\rho)$ we may assume that $N := \rho L^n$ is an integer. Let $k \in \mathbb{N}$ and put $L' = k(L + R).$ We can place $M := k^n$ copies of the box $\Lambda_L$ inside the larger box $\Lambda_{L'}$ with separation $R$ between neighboring boxes. From an $N$-particle trial state $\Psi$ in $\Lambda_L$ we can construct a trial state with $MN$ particles by placing independent particles in each of the $M$ boxes, each with state $\Psi$. Because of the Dirichlet boundary condition, this gives a trial state on $\Lambda_{L'}$ by extending $\Psi$ by zero and, due to the separation, particles in different boxes do not interact. Minimizing over $\Psi$ yields

$$e_L(\rho) \geq (1 + R/L)^n e_{L'}(\rho[1 + R/L]^{-n}).$$

This estimate holds for each $k \in \mathbb{N}$, so the result follows by taking the limit $k \to \infty$. □

By Lemma A.2, we have

$$e_L(\rho) - \mu \rho \geq e(\rho_L) - \mu \rho$$

$$= [1 + R/L]^n (e(\rho_L) - \mu \rho_L) + \varepsilon_L$$

$$\geq [1 + R/L]^n f(\mu) + \varepsilon_L,$$

where

$$\rho_L := \rho[1 + R/L]^{-n} \quad \text{and} \quad \varepsilon_L := e(\rho_L)(1 - [1 + R/L]^n).$$

Now notice that, by (A.4),

$$f_L(\mu) = \inf_{\rho \in [0, \rho_\mu]} [e_L(\rho) - \mu \rho],$$

for some $\rho_\mu > 0$. From the upper bound (A.1), we then have

$$f_L \geq [1 + R/L]^n f(\mu) + C\rho_\mu^2 (1 - [1 + R/L]^n),$$

and consequently

$$\liminf_{L \to \infty} f_L(\mu) \geq f(\mu),$$

as desired.

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