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The Ground State Energy of the Weakly Interacting Bose Gas at High Density

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Abstract We prove the Lee-Huang-Yang formula for the ground state energy of the 3D Bose gas with repulsive interactions described by the exponential function, in a simultaneous limit of weak coupling and high density. In particular, we show that the Bogoliubov approximation is exact in an appropriate parameter regime, as far as the ground state energy is concerned.

Keywords Repulsive Bose gas · Ground state energy · Lee-Huang-Yang formula · Bogoliubov's approximation

1 Introduction

We consider a three dimensional system of N interacting bosons in a cubic (periodic) box Λ of side length L, described by the Hamiltonian:

$$H_N = -\sum_{i=1}^{N} \Delta_i + \frac{a_0}{R_0^3} \sum_{1\le i<j\le N} v_{R_0}(\mathbf{x}_i - \mathbf{x}_j). \tag{1.1}$$

Here $\mathbf{x}_i \in \Lambda$, $i = 1, \ldots, N$, are the positions of the particles, and Δ_i denotes the Laplacian with respect to $\mathbf{x}_i$. Units are chosen such that $\hbar = 2m = 1$, where m is the mass of the particles. The interaction potential is taken to be $v_{R_0}(\mathbf{x}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} e^{-|\mathbf{x}+\mathbf{n}L|/R_0}$, and a_0 and R_0 are positive constants. The Hamiltonian (1.1) operates on symmetric wave functions in the Hilbert space $L^2(\Lambda^N, d\mathbf{x}_1 \cdots d\mathbf{x}_N)$, as is appropriate for bosons.

Dedicated with best wishes to Édouard Brézin and to Giorgio Parisi on the occasion of their 70th and 60th birthdays.

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We are interested in the ground state energy $E_0(N)$ of (1.1) in the thermodynamic limit when N and $|\Lambda|$ tend to infinity with the density $\rho = N/|\Lambda|$ fixed, and in a weak coupling regime $a_0 \ll \min\{\rho^{-1/3}, R_0\}$. The constant a_0 is the first Born approximation to the scattering length a of the potential $(a_0/R_0^3)e^{-|\mathbf{x}|/R_0}$, which is defined as usual as $a = \lim_{|\mathbf{x}|\to\infty} |\mathbf{x}|(1-\psi_0(\mathbf{x}))$, with ψ_0 a solution to the zero energy scattering equation

$$-2\Delta\psi(\mathbf{x}) + \frac{a_0}{R_0^3} e^{-|\mathbf{x}|/R_0}\psi(\mathbf{x}) = 0 \tag{1.2}$$

with boundary condition $\lim_{|\mathbf{x}|\to\infty}\psi(\mathbf{x}) = 1$. It is well known that, if $a_0/R_0 \ll 1$, a/a_0 can be written in terms of a convergent series in powers of a_0/R_0 (Born series), which will be denoted by $a = a_0 + \sum_{k\geq 1} a_k$, and whose first non-trivial term is given by

$$a_1 = -\frac{1}{128\pi^3}\int_{\mathbb{R}^3} d\mathbf{k} \frac{\nu(\mathbf{k})^2}{\mathbf{k}^2} = -\frac{5\pi}{16}\frac{a_0^2}{R_0}, \tag{1.3}$$

where

$$\nu(\mathbf{k}) = \frac{a_0}{R_0^3}\int_{\mathbb{R}^3} d\mathbf{x}\, e^{-|\mathbf{x}|/R_0} e^{-i\mathbf{k}\mathbf{x}} = \frac{8\pi a_0}{[1+(\mathbf{k}R_0)^2]^2}. \tag{1.4}$$

The current understanding of the properties of the ground state of (1.1) is based on the pioneering work of Bogoliubov [1], who developed an approximate theory of the ground state of weakly repulsive bosons. In the regime $1 \gg a/R_0 \gg \sqrt{\rho a^3} \gg (a/R_0)^2$, Bogoliubov's theory predicts [8] that the ground state energy $E_0(N)$ of (1.1) in the thermodynamic limit $N, |\Lambda| \to \infty$, with $\rho = N/|\Lambda|$ fixed, satisfies

$$\lim_{N,|\Lambda|\to\infty} \frac{E_0(N)}{N} = 4\pi\rho a\left(1 + \frac{128}{15\sqrt{\pi}}\sqrt{\rho a^3} + o\big(\sqrt{\rho a^3}\big)\right). \tag{1.5}$$

This formula was first derived in [2, 3] and it is known as the Lee-Huang-Yang formula. Our goal is to prove that the expression (1.5) is asymptotically correct in a regime such that $a \ll \rho^{-1/3} \ll R_0$, that is a *weak coupling* and *high density* regime. We shall prove the following theorem.

Theorem 1 *Let $Y = \rho a^3$. There exists a positive constant d_0, which can be chosen to be $d_0 = 1/69$, such that, if $0 < d < d_0$ and $a/R_0 = O(Y^{1/2-d})$, then (1.5) is valid, asymptotically as $Y \to 0$.*

This result represents the first rigorous proof of the Lee-Huang-Yang formula for the ground state energy of a weak-coupling Bose gas. We note that for $d < 1/6$, $R_0^3\rho \gg 1$ and hence Theorem 1 concerns the high density regime. Our result is not expected to be optimal. In fact, the formula (1.5) is expected to hold even for $d = 1/2$, i.e., for a/R_0 fixed and $\rho a^3 \to 0$ [2, 3], but the Bogoliubov approximation is not valid in this case. The prediction of Bogoliubov's theory is that (1.5) should be valid for any $0 < d < 1/4$, i.e., in the regime $a/R_0 \gg \sqrt{\rho a^3} \gg (a/R_0)^2$. The latter condition is necessary in order that $a \approx a_0 + a_1$ to the desired accuracy (i.e., up to error terms that are much smaller than $a_0\rho\sqrt{\rho a_0^3}$), and the former is certainly needed since $E_0(N)/N \leq 4\pi\rho a_0$ (i.e., the right side of (1.5) must be equal to $4\pi\rho a_0$ plus a *negative* correction, which requires $|a_1| \gg a_0\sqrt{\rho a_0^3}$).

For simplicity, we shall restrict our attention to interaction potentials given by the exponential function. Our proof can be adapted to a larger class of potentials, including the

Yukawa potential. In our proof, however, we need the potential to be positive definite, with a Fourier transform satisfying nice decay properties as $|\mathbf{k}| \to \infty$ (e.g., polynomial decay), and our proof does not immediately extend beyond this class. Such restrictive condition is not supposed to have any physical relevance, of course, and (1.5) should hold for much more general repulsive potentials. We hope that the technical restrictions under which we proved Theorem 1 will be eliminated in future works.[1]

The proof of Theorem 1 will proceed in two steps: we will get upper and lower bounds with the correct asymptotic form. The proof of the upper bound is based on a computation of the variational energy corresponding to the Bogoliubov trial wave function, following ideas of Girardeau and Arnowitt [6], see the next section.

The strategy of the proof of a lower bound will follow closely the one of Lieb and Solovej in [7], where the ground state energy of bosonic jellium was investigated. We shall first localize the Hamiltonian in boxes of size ℓ. Using the positivity of the Fourier transform of the exponential interaction, we shall derive a preliminary estimate on the ground state energy and, correspondingly, on the degree of condensation in the small boxes. With this a priori bound on the number of particles n_+ outside the condensate, we shall be able to bound from below the full Hamiltonian by the Bogoliubov Hamiltonian minus an error term, depending on the a priori bound on n_+. The key point is that it is possible to find a scaling regime for a_0 and R_0 such that the new error term is much smaller than the preliminary one, as $Y \to 0$. With this improved bound on the ground state energy we shall obtain new improved bounds on the size of fluctuations of n_+ that, in combination with the bounds for the ground state energy, will allow us to conclude the desired lower bound.

2 The Upper Bound

Let us first derive an upper bound to the ground state energy, asymptotically agreeing with (1.5). In second quantized form, the Hamiltonian H_N can be rewritten as:

$$H_N = \sum_{\mathbf{k}} \mathbf{k}^2 c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + \frac{1}{2|\Lambda|} \sum_{\mathbf{k},\mathbf{q},\mathbf{p}} v(\mathbf{p}) c_{\mathbf{k}+\mathbf{p}}^\dagger c_{\mathbf{q}-\mathbf{p}}^\dagger c_{\mathbf{k}} c_{\mathbf{q}}, \tag{2.1}$$

where the sums run over vectors of the form $2\pi \boldsymbol{\nu}/L$, $\boldsymbol{\nu} \in \mathbb{Z}^3$, and $c_{\mathbf{k}}^\dagger$, $c_{\mathbf{k}}$ are standard bosonic creation and annihilation operators, associated with the canonical basis of plane waves (for an introduction, see, e.g., [8]). Following [6], we choose the following variational state, inspired by Bogoliubov's approximate treatment of the weak coupling Bose gas:

$$|\Omega_{B,N}\rangle = \exp\left\{\frac{1}{2}\sum_{\mathbf{k}\neq\mathbf{0}} \psi(\mathbf{k})\big(\beta_{\mathbf{0}}^\dagger \alpha_{\mathbf{k}} - \beta_{\mathbf{0}} \alpha_{\mathbf{k}}^\dagger\big)\right\}|\Omega_N\rangle \tag{2.2}$$

where:

(1) $|\Omega_N\rangle = (N!)^{-1/2}(c_{\mathbf{0}}^\dagger)^N|0\rangle$ is the ground state for N non-interacting particles;
(2) the operator $\alpha_{\mathbf{k}}$ is the pair annihilation operator $\alpha_{\mathbf{k}} = c_{\mathbf{k}} c_{-\mathbf{k}}$;

[1] In the process of writing up this paper, we learned that E.H. Lieb and J.P. Solovej managed to prove the analogue of Theorem 1 for a larger class of repulsive potentials and in the larger regime $0 < d < 1/6 + \epsilon$ for some $\epsilon > 0$. We thank them for communicating their results to us.

(3) if we denote by $N_{\mathbf{0}} = c_{\mathbf{0}}^{\dagger} c_{\mathbf{0}}$ the number operator associated to the constant wave function, $\beta_{\mathbf{0}}$ is the partial isometry defined by

$$\beta_{\mathbf{0}}^{1/2} = c_{\mathbf{0}} N_{\mathbf{0}}^{-1/2}, \tag{2.3}$$

having the properties

$$\begin{aligned} &\beta_{\mathbf{0}}|\Omega_N\rangle = |\Omega_{N-2}\rangle \quad (N \geq 2), \qquad \beta_{\mathbf{0}}^{\dagger}|\Omega_N\rangle = |\Omega_{N+2}\rangle, \\ &[\beta_{\mathbf{0}}, N_{\mathbf{0}}] = 2\beta_{\mathbf{0}}, \qquad [\beta_{\mathbf{0}}^{\dagger}, N_{\mathbf{0}}] = -2\beta_{\mathbf{0}}^{\dagger}, \\ &[\beta_{\mathbf{0}}, c_{\mathbf{k}}] = [\beta_{\mathbf{0}}, c_{\mathbf{k}}^{\dagger}] = 0 \quad (\mathbf{k} \neq \mathbf{0}); \end{aligned} \tag{2.4}$$

(4) ψ is a continuous function from $\mathbb{R}^3$ to $\mathbb{R}$.

Note that $|\Omega_{B,N}\rangle$ is normalized, and that the particle number is equal to N. The variational principle implies the upper bound

$$E_0(N) \leq \langle \Omega_{B,N}|H_N|\Omega_{B,N}\rangle. \tag{2.5}$$

Following [6], after a lengthy but straightforward computation, we find that in the thermodynamic limit

$$\begin{aligned} \lim_{N\to\infty} \frac{1}{N}\langle \Omega_{B,N}|H_N|\Omega_{B,N}\rangle &= \frac{1}{2}\rho\nu(\mathbf{0}) + \rho^{-1}\int \frac{d\mathbf{k}}{(2\pi)^3}\left[\mathbf{k}^2 + \rho_0\nu(\mathbf{k}) + \frac{1}{2}I_2(\mathbf{k})\right]\sinh^2\psi(\mathbf{k}) \\ &\quad - \rho^{-1}\int \frac{d\mathbf{k}}{(2\pi)^3}\left[\rho_0\nu(\mathbf{k}) - \frac{1}{2}I_1(\mathbf{k})\right]\sinh\psi(\mathbf{k})\cosh\psi(\mathbf{k}), \end{aligned} \tag{2.6}$$

where:

$$\begin{aligned} \rho_0 &= \rho - \int \frac{d\mathbf{q}}{(2\pi)^3}\sinh^2\psi(\mathbf{q}), \\ I_1(\mathbf{k}) &= \int \frac{d\mathbf{q}}{(2\pi)^3}\nu(\mathbf{k}-\mathbf{q})\sinh\psi(\mathbf{q})\cosh\psi(\mathbf{q}), \\ I_2(\mathbf{k}) &= \int \frac{d\mathbf{q}}{(2\pi)^3}\nu(\mathbf{k}-\mathbf{q})\sinh^2\psi(\mathbf{q}). \end{aligned} \tag{2.7}$$

Choosing $\psi(\mathbf{k}) = \frac{1}{2}\tanh^{-1}\frac{\rho\nu(\mathbf{k})}{\mathbf{k}^2+\rho\nu(\mathbf{k})}$, we find that

$$\begin{aligned} \sinh^2\psi(\mathbf{k}) &= \frac{1}{2}\frac{\mathbf{k}^2 + \rho\nu(\mathbf{k}) - \sqrt{\mathbf{k}^4 + 2\rho\nu(\mathbf{k})\mathbf{k}^2}}{\sqrt{\mathbf{k}^4 + 2\rho\nu(\mathbf{k})\mathbf{k}^2}}, \\ \sinh\psi(\mathbf{k})\cosh\psi(\mathbf{k}) &= \frac{1}{2}\frac{\rho\nu(\mathbf{k})}{\sqrt{\mathbf{k}^4 + 2\rho\nu(\mathbf{k})\mathbf{k}^2}}. \end{aligned} \tag{2.8}$$

Recall that $\nu(\mathbf{k})$ is given in (1.4), and that $a/R_0 = O(Y^{1/2-d})$. A simple calculation shows that

$$\rho_0 = \rho\big(1 + O(\sqrt{\rho a^3})\big) \tag{2.9}$$

for any $d > 0$. Moreover, we have the bounds

$$|I_1(\mathbf{k})| \le C\rho a_0 \frac{a_0}{R_0} \frac{1}{[1+(\mathbf{k}R_0)^2]^2}, \qquad |I_2(\mathbf{k})| \le C\rho a_0 \sqrt{\rho a_0^3} \frac{1}{[1+(\mathbf{k}R_0)^2]^2} \tag{2.10}$$

for a suitable constant C. Substituting these bounds into (2.6) we find that

$$\begin{aligned} &\frac{1}{4\pi\rho a_0} \lim_{N\to\infty} \frac{1}{N} \langle \Omega_{B,N} | H_N | \Omega_{B,N} \rangle \\ &\quad = 1 - \frac{1}{2\pi\rho^2 a_0} \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \left(\mathbf{k}^2 + \rho v(\mathbf{k}) - \sqrt{\mathbf{k}^4 + 2\rho v(\mathbf{k})\mathbf{k}^2} \right) + o(\sqrt{\rho a^3}) \end{aligned} \tag{2.11}$$

for $0 < d < 1/4$. A computation [8] shows that for $d > 0$ the integral on the right side equals

$$\frac{a_1}{a_0} + \frac{128}{15\sqrt{\pi}} \sqrt{\rho a_0^3} + o(\sqrt{\rho a^3}). \tag{2.12}$$

Noting that $a/(a_0 + a_1) = O(a_0/R_0)^2 \ll Y^{1/2}$ for $d < 1/4$ this yields the desired result.

Remark The upper bound we have just derived yields the desired expression for any $0 < d < 1/4$. By suitably modifying the trial function $\psi(\mathbf{k})$ above, one can actually show that the upper bound holds for any $0 < d < 1/2$ [4]. For $d = 1/2$, however, the ansatz (2.2) can not be expected to yield the Lee-Huang-Yang formula, even for the optimal choice of ψ.

3 The Lower Bound

We shall split the lower bound into several parts. The strategy is similar to the proof of the lower bound on the ground state energy of jellium by Lieb and Solovej in [7], and we shall refer to their paper for several essential ingredients.

3.1 Sliding and Localizing

We start by rewriting (1.1) in the form

$$\begin{aligned} H_N' = H_N - 4\pi N\rho a_0 = &-\sum_{i=1}^N \Delta_i + \frac{a_0}{R_0^3} \Bigg[\sum_{1\le i<j\le N} v_{R_0}(\mathbf{x}_i - \mathbf{x}_j) \\ &- \rho \sum_{i=1}^N \int_\Lambda d\mathbf{y}\, v_{R_0}(\mathbf{x}_i - \mathbf{y}) + \frac{\rho^2}{2} \iint_{\Lambda\times\Lambda} d\mathbf{x}\, d\mathbf{y}\, v_{R_0}(\mathbf{x} - \mathbf{y}) \Bigg], \end{aligned} \tag{3.1}$$

with $\rho = N/|\Lambda|$. We shall use the sliding method of [5] to reduce the problem to a small box.

Let t, with $0 < t < 1/2$, be a parameter which we shall choose later to depend on ρ in such a way that $t \to 0$ as $\rho R_0^3 \to \infty$. Let $\chi \in C_0^\infty(\mathbb{R}^3)$ be supported in $[(-1+t)/2, (1-t)/2]^3$, $0 \le \chi \le 1$, with $\chi(\mathbf{x}) = 1$ for $\mathbf{x}$ in the smaller box $[(-1+2t)/2, (1-2t)/2]^3$, and $\chi(\mathbf{x}) = \chi(-\mathbf{x})$. Assume that all m-th order derivatives of χ are bounded by $C_m t^{-m}$, where the constants C_m depend only on m and are, in particular, independent of t. If $M \in \mathbb{N}$ and $\ell = M^{-1}L$, let $\chi_\ell(\mathbf{x})$ be a function on the torus Λ defined by $\chi_\ell(\mathbf{x}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} \chi(\ell^{-1}(\mathbf{x} + \mathbf{n}L))$. For given χ we also define $\gamma > 0$ by $\gamma^{-1} = \int \chi(\mathbf{y})^2\, d\mathbf{y}$, and note that $1 \le \gamma \le (1-2t)^{-3}$. We shall prove the following.

Lemma 3.1 *Let $\ell t R_0^{-1}$ be large enough. There exists a function of the form $\omega(t) = \text{const}\, t^{-1} R_0/\ell$ such that if we set $R^{-1} = R_0^{-1} + \omega(t)/\ell$ and*

$$w_R^\Lambda(\mathbf{x}, \mathbf{y}) = \chi_\ell(\mathbf{x}) v_R(\mathbf{x} - \mathbf{y}) \chi_\ell(\mathbf{y}) \tag{3.2}$$

then the potential energy satisfies

$$\begin{aligned} &\sum_{1 \le i < j \le N} v_{R_0}(\mathbf{x}_i - \mathbf{x}_j) - \rho \sum_{i=1}^N \int_\Lambda d\mathbf{y} v_{R_0}(\mathbf{x}_i - \mathbf{y}) + \frac{\rho^2}{2} \iint_{\Lambda\times\Lambda} d\mathbf{x}\, d\mathbf{y} v_{R_0}(\mathbf{x} - \mathbf{y}) \\ &\ge \frac{\gamma R}{R_0} \sum_{\mathbf{m} \in [1,\dots,M]^3} \int_{Q_\mathbf{m}} \frac{d\mathbf{z}}{\ell^3} \Bigg\{ \sum_{1 \le i < j \le N} w_R^\Lambda(\mathbf{x}_i + \mathbf{z}, \mathbf{x}_j + \mathbf{z}) - \rho \sum_{j=1}^N \int_\Lambda d\mathbf{y} w_R^\Lambda(\mathbf{x}_j + \mathbf{z}, \mathbf{y} + \mathbf{z}) \\ &\quad + \frac{1}{2}\rho^2 \iint_{\Lambda\times\Lambda} d\mathbf{x}\, d\mathbf{y}\, w_R^\Lambda(\mathbf{x} + \mathbf{z}, \mathbf{y} + \mathbf{z}) \Bigg\} - N \frac{\omega(t) R}{2\ell} - \text{const}\, N^2 e^{-L/(2R)}, \end{aligned} \tag{3.3}$$

where $Q_\mathbf{m}$ is a cube of side length ℓ and centered at $\mathbf{m}\ell$ (so that the collection $\{Q_\mathbf{m}\}_{\mathbf{m} \in [1,\dots,M]^3}$ paves the torus Λ).

The proof of Lemma 3.1 utilizes the following lemma, whose proof will be given after the proof of Lemma 3.1. An analogous result for the Yukawa interaction potential was proved in [5, Lemma 2.1].

Lemma 3.2 *Let $K : \mathbb{R}^3 \to \mathbb{R}$ be given by*

$$K(\mathbf{z}) = e^{-\nu|\mathbf{z}|} \left(1 - \frac{e^{-\omega|\mathbf{z}|}}{1 + \omega/\nu} h(\mathbf{z}) \right) \tag{3.4}$$

with $\nu \ge \omega > 0$. Let h satisfy (i) *h is a C^6 function of compact support*; (ii) $h(0) = 1$; (iii) *all its m-th order derivatives*, $1 \le m \le 6$, *are bounded by Ct^{1-m} for some constants $C > 0$ and $t > 0$. Assume further that $h(\mathbf{z}) = h(-\mathbf{z})$ so that K has a real Fourier transform. There exists a constant C_1 (depending only on C but not on t, ω or ν) such that, if* $\min\{1, \omega\}\nu t \ge C_1$, *then K has a positive Fourier transform.*

Proof of Lemma 3.1 We calculate

$$\begin{aligned} &\frac{\gamma R}{R_0} \sum_{\mathbf{m} \in [1,\dots,M]^3} \int_{Q_\mathbf{m}} \frac{d\mathbf{z}}{\ell^3} w_R^\Lambda(\mathbf{x} + \mathbf{z}, \mathbf{y} + \mathbf{z}) \\ &\quad = \frac{\gamma R}{R_0} \int_\Lambda \frac{d\mathbf{z}}{\ell^3} \chi_\ell(\mathbf{x} + \mathbf{z}) v_R(\mathbf{x} - \mathbf{y}) \chi_\ell(\mathbf{y} + \mathbf{z}) = \frac{R}{R_0} h_\ell(\mathbf{x} - \mathbf{y}) v_R(\mathbf{x} - \mathbf{y}), \end{aligned} \tag{3.5}$$

where we have set $h_\ell = \gamma \ell^{-3} \chi_\ell * \chi_\ell$. Note that $h_\ell(\mathbf{x})$ vanishes if $\|\mathbf{x}\| \ge \ell$, so we can naturally introduce a function $h : \mathbb{R}^3 \to \mathbb{R}$ of compact support and vanishing outside the cube of side 2 centered at the origin, such that $h_\ell(\mathbf{x}) = \sum_{\mathbf{n} \in \mathbb{Z}^3} h(\ell^{-1}(\mathbf{x} + \mathbf{n}L))$. Note that: (i) $h(\mathbf{0}) = 1$; (ii) h has a quadratic maximum at $\mathbf{z} = \mathbf{0}$; (iii) h is an even C^∞ function of compact support; (iv) all m-th order derivatives of h, $m \ge 1$, are bounded by $C_m t^{1-m}$, where the constants C_m depend only on m and are, in particular, independent of t. The function h thus satisfies all the hypothesis of Lemma 3.2. Note also that the role of ν and ω in Lemma 3.2

are here played by ℓR_0^{-1} and $\omega(t)$ respectively. So, if $\omega(t) \geq C_1 R_0 \ell^{-1} t^{-1}$, where C_1 is the constant appearing in the statement of Lemma 3.2, we then conclude from it that the Fourier transform of the function $K(\mathbf{x}) = e^{-|\mathbf{x}|/R_0} - h(\ell^{-1}\mathbf{x})e^{-|\mathbf{x}|/R}(R/R_0)$, is positive. Now, defining $K^\Lambda(\mathbf{x}) = \sum_{\mathbf{n}\in\mathbb{Z}^3} K(\mathbf{x}+\mathbf{n}L)$ and $\varphi(\mathbf{x}) = v_{R_0}(\mathbf{x}) - h_\ell(\mathbf{x})v_R(\mathbf{x})(R/R_0)$, we note that $\varphi(\mathbf{x}) = K^\Lambda(\mathbf{x}) + R(\mathbf{x})$, with $|R(\mathbf{x})| \leq \text{const}\, e^{-(L-\ell)/R}$. Because of positivity of the Fourier transform of K,

$$\sum_{1\leq i<j\leq N} \varphi(\mathbf{x}_i - \mathbf{x}_j) - \rho \sum_{j=1}^{N} \int_\Lambda \varphi(\mathbf{x}_i - \mathbf{y}) + \frac{1}{2}\rho^2 \iint_{\Lambda\times\Lambda} \varphi(\mathbf{x}-\mathbf{y})\, d\mathbf{x}\, d\mathbf{y}$$
$$\geq -\frac{N}{2} K^\Lambda(\mathbf{0}) - \text{const}\, N^2 e^{-(L-\ell)/R}. \tag{3.6}$$

Since $K^\Lambda(\mathbf{0}) \leq R\omega/\ell + \text{const}\exp(-L/R_0)$ this implies (3.3). □

Proof of Lemma 3.2 We write $h(\mathbf{z}) = 1 + q(\mathbf{z}) + F(\mathbf{z})$, where $q(\mathbf{z})$ is an even polynomial of degree 4 that vanishes at the origin, and $F(\mathbf{z}) \leq Ct^{-5}|\mathbf{z}|^6$. The Fourier transform of $e^{-\nu|\mathbf{z}|} - e^{-(\nu+\omega)|\mathbf{z}|}/(1+\omega/\nu)$ is given by

$$\frac{8\pi\nu}{(\nu^2+\mathbf{p}^2)^2} - \frac{8\pi\nu}{((\nu+\omega)^2+\mathbf{p}^2)^2} \geq \frac{48\pi\nu^2\omega}{((\nu+\omega)^2+\mathbf{p}^2)^3}. \tag{3.7}$$

Moreover, the Fourier transform of $q(\mathbf{z})e^{-(\nu+\omega)|\mathbf{z}|}$ is

$$q(i\nabla_{\mathbf{p}})\frac{8\pi(\nu+\omega)}{((\nu+\omega)^2+\mathbf{p}^2)^2} \tag{3.8}$$

whose absolute value, if $\nu t \geq C_1$, can be bounded above by const $\cdot\, \nu t^{-1}[(\nu+\omega)^2+\mathbf{p}^2]^{-3}$ (here we used that q is assumed to be even and that its m'th order coefficients are bounded by Ct^{1-m}). Finally, we claim that the Fourier transform of $F(\mathbf{z})e^{-(\nu+\omega)|\mathbf{z}|}$ is bounded by const $\cdot\, \nu^{-3}t^{-5}[(\nu+\omega)^2+\mathbf{p}^2]^{-3}$. To see this, note that $F(\mathbf{z})e^{-(\nu+\omega)|\mathbf{z}|}$ is a C^6 function, and hence

$$\left((\nu+\omega)^2+\mathbf{p}^2\right)^3 \int F(\mathbf{z})e^{-(\nu+\omega)|\mathbf{z}|}e^{-i\mathbf{p}\cdot\mathbf{z}}d\mathbf{z} = \int \left[\left((\nu+\omega)^2-\Delta\right)^3 F(\mathbf{z})e^{-(\nu+\omega)|\mathbf{z}|}\right]e^{-i\mathbf{p}\cdot\mathbf{z}}d\mathbf{z}. \tag{3.9}$$

It is not difficult to see that the latter integral is bounded by $Ct^{-5}\nu^{-3}$. After collecting all the terms, we arrive at the statement of the lemma. □

Below, we shall choose the parameters t and ℓ as functions of ρ, R_0 and a_0. We shall choose them in such a way that $t \ll 1$ and $\ell \gg R_0$. Moreover, we will have conditions of the form

$$\frac{\ell t}{R_0} \to \infty, \qquad \frac{a_0}{R_0^2}\frac{\omega(t)}{\ell}\frac{1}{\rho a_0\sqrt{\rho a_0^3}} \to 0, \quad \text{and} \quad \frac{R}{R_0} \to 1 \tag{3.10}$$

as $\rho a_0^3 \to 0$, such that the error in the specific ground state energy corresponding to the term $N\omega(t)R/(2\ell)$ in (3.3) is much smaller than $N\rho a_0\sqrt{\rho a_0^3}$, which is the precision to which we want to compute the ground state energy.

Consider now the n-particle Hamiltonian

$$H^n_{\mathbf{m},\mathbf{z}} = -\sum_{j=1}^n \Delta^{(j)}_{Q_{\mathbf{m},\mathbf{z}}} + \frac{\gamma a_0 R}{R_0^4} W_{\mathbf{z}}, \tag{3.11}$$

where we have introduced the Neumann Laplacian $\Delta^{(j)}_{Q_{\mathbf{m},\mathbf{z}}}$ in the cube $Q_{\mathbf{m},\mathbf{z}} = Q_{\mathbf{m}} + \mathbf{z}$ and the potential

$$\begin{aligned} W_{\mathbf{z}}(\mathbf{x}_1, \ldots, \mathbf{x}_n) &= \sum_{1\le i<j\le n} w_R^\Lambda(\mathbf{x}_i + \mathbf{z}, \mathbf{x}_j + \mathbf{z}) - \rho \sum_{j=1}^n \int_\Lambda d\mathbf{y}\, w_R^\Lambda(\mathbf{x}_j + \mathbf{z}, \mathbf{y} + \mathbf{z}) \\ &\quad + \frac{1}{2}\rho^2 \iint_{\Lambda\times\Lambda} d\mathbf{x}\, d\mathbf{y}\, w_R^\Lambda(\mathbf{x} + \mathbf{z}, \mathbf{y} + \mathbf{z}). \end{aligned} \tag{3.12}$$

Denoting by $E^n_{\mathbf{m},\mathbf{z}}$ the ground state energy of the Hamiltonian $H^n_{\mathbf{m},\mathbf{z}}$ in (3.11) considered as a bosonic Hamiltonian for n particles confined to the cube $Q_{\mathbf{m},\mathbf{z}}$, and using Lemma 3.1, we find that the ground state energy E_0 of (1.1) can be bounded below by

$$E_0 \ge 4\pi N\rho a_0 + \sum_{\mathbf{m}\in[1,\ldots,M]^3} \int_{Q_{\mathbf{m}}} \frac{d\mathbf{z}}{\ell^3} \inf_{1\le n\le N} E^n_{\mathbf{m},\mathbf{z}} - N\frac{a_0\omega(t)R}{2\ell R_0^3} - \text{const}\, N^2 \frac{a_0}{R_0^3} e^{-L/(2R)}. \tag{3.13}$$

Note that all the Hamiltonians $H^n_{\mathbf{m},\mathbf{z}}$ are unitarily equivalent to

$$\begin{aligned} &-\sum_{j=1}^n \Delta^{(j)}_\ell + \frac{\gamma a_0 R}{R_0^4}\Bigg[\sum_{1\le i<j\le n} w_R^\Lambda(\mathbf{x}_i, \mathbf{x}_j) - \rho\sum_{j=1}^n \int_\Lambda d\mathbf{y} w_R^\Lambda(\mathbf{x}_j, \mathbf{y}) \\ &\quad + \frac{1}{2}\rho^2 \iint_{\Lambda\times\Lambda} d\mathbf{x}\, d\mathbf{y}\, w_R^\Lambda(\mathbf{x}, \mathbf{y})\Bigg] \end{aligned} \tag{3.14}$$

where $\Delta^{(j)}_\ell$ denotes the Neumann Laplacian for the j-th particle in the cube $[-\ell/2, \ell/2]^3$. As a consequence, in the $L \to \infty$ limit, we have reduced the problem to studying the Hamiltonians H^n_ℓ on $L^2([-\ell/2, \ell/2]^{3n})$, given by

$$\begin{aligned} H^n_\ell &= -\sum_{j=1}^n \Delta^{(j)}_\ell + \frac{\gamma a_0 R}{R_0^4}\Bigg[\sum_{1\le i<j\le n} w_R(\mathbf{x}_i, \mathbf{x}_j) - \rho\sum_{j=1}^n \int_{\mathbb{R}^3} d\mathbf{y}\, w_R(\mathbf{x}_j, \mathbf{y}) \\ &\quad + \frac{1}{2}\rho^2 \iint_{\mathbb{R}^3\times\mathbb{R}^3} d\mathbf{x}\, d\mathbf{y}\, w_R(\mathbf{x}, \mathbf{y})\Bigg] \end{aligned} \tag{3.15}$$

with $w_R(\mathbf{x}, \mathbf{y}) = \chi(\mathbf{x}\ell^{-1}) e^{-|\mathbf{x}-\mathbf{y}|/R} \chi(\mathbf{y}\ell^{-1})$. If E^n_ℓ is the ground state energy of H^n_ℓ, from (3.13) we infer that

$$\lim_{N\to\infty} \frac{E_0}{N} \ge 4\pi\rho a_0 + \frac{1}{\rho\ell^3} \inf_n E^n_\ell - \frac{a_0\omega(t)R}{2\ell R_0^3}. \tag{3.16}$$

In the remainder of this paper we shall study the Hamiltonians (3.15). For future reference, let us finally note that in second quantized form H_ℓ^n can be rewritten as

$$H_\ell^n = \sum_{\mathbf{p}} \mathbf{p}^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{\gamma a_0 R}{R_0^4}\left[\frac{1}{2}\sum_{\mathbf{pq},\boldsymbol{\mu\nu}} \hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\boldsymbol{\nu}} - \rho\ell^3 \sum_{\mathbf{pq}} \hat{w}_{\mathbf{0p},\mathbf{0q}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}} + \frac{1}{2}\rho^2\ell^6 \hat{w}_{\mathbf{00},\mathbf{00}}\right] \tag{3.17}$$

where the sums over the momenta run over the values $\mathbf{p} = (p_1, p_2, p_3)$ such that $\ell p_i/\pi \in \mathbb{Z}_+$, $a_{\mathbf{p}}^\dagger$, $a_{\mathbf{p}}$ are bosonic creation/annihilation operators corresponding to the orthonormal basis $\phi_{\mathbf{p}}(\mathbf{x}) = c_{\mathbf{p}}\ell^{-3/2}\prod_{j=1}^3 \cos(p_j\pi\ell^{-1}(x_j + \ell/2))$, and the coefficients $\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}}$ are defined as

$$\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} = \iint d\mathbf{x}\, d\mathbf{y}\, w_R(\mathbf{x},\mathbf{y})\phi_{\mathbf{p}}(\mathbf{x})\phi_{\mathbf{q}}(\mathbf{y})\phi_{\boldsymbol{\mu}}(\mathbf{x})\phi_{\boldsymbol{\nu}}(\mathbf{y}). \tag{3.18}$$

3.2 Scalings

Before proceeding with the proof of the lower bound, let us make a few remarks on the choice of the parameters a_0, R_0, ℓ, t. We recall that our purpose is to compute the ground state energy of (1.1) up to terms of the order $N\rho a_0\sqrt{\rho a_0^3}$, asymptotically as $Y = \rho a_0^3 \to 0$. In the following we shall choose $a_0/R_0 \sim Y^{1/2-d}$, $a_0/\ell \sim Y^{b+1/2}$ and $t \sim Y^\tau$, where d, b and τ are positive scaling exponents. [Here by $f \sim g$ we mean that $C^{-1}g \le f \le Cg$, for some universal constant C.] We shall require $d < 1/4$. Note that the conditions $b, d > 0$ and $d < 1/4$ imply in particular that $a_0 \ll R_0 \ll \ell$ and $a_0/\ell \ll \sqrt{\rho a_0^3}$ (two conditions that are of course necessary to be able to neglect finite size effects due to the boxes of size ℓ) and that $a_0/R_0 \gg \sqrt{\rho a_0^3} \gg (a_0/R_0)^2$ (a condition that is necessary for the Bogoliubov approximation to be valid, as explained in the Introduction). In order to be able to prove that the various error terms in our estimates are much smaller than $N\rho a_0\sqrt{\rho a_0^3}$ we will be forced to require that b, d, τ are small enough and that they satisfy a number of inequalities, some of which will now be discussed. Such inequalities will be satisfied by proper choices of b and τ, as long as d is small enough.

1. We require $\rho R_0^3 \gg 1$, that is $0 < d < 1/6$. Note that under this condition we also have $a_0/R_0 \gg \sqrt{\rho a_0^3} \gg (a_0/R_0)^3$.
2. We require $\ell t R_0^{-1} \gg 1$, as in (3.10), so that $b + d > \tau$.
3. We require $a_0 R_0^{-1}\ell^{-2}t^{-1} \ll \rho a_0\sqrt{\rho a_0^3}$, as in (3.10), so that $2b - d - \tau > 0$.
4. Noting that the contribution from the potential energy per particle in H_ℓ^n is expected (on the basis of Bogoliubov theory) to be of order $na_0R_0^{-1}$ relative to the main term, we require both that $ta_0R_0^{-1}$ and $a_0(R^{-1} - R_0^{-1})$ are much smaller than $\sqrt{\rho a_0^3}$, in order to guarantee that the errors produced by the presence of γ in front of the potential energy and by the replacement of R_0 with R are negligible. These conditions imply $\tau > d$ and $2b + d > \tau$.

Further requirements will be discussed below.

3.3 A Priori Bounds on n and n_+

As a first step in our argument, we shall derive preliminary bounds on the number of particles minimizing E_ℓ^n and on the average number of particles $\langle\hat{n}_+\rangle$ outside the condensate. [Here the operator $\hat{n}_+$ is defined, in second quantized form, as $\hat{n}_+ = \sum_{\mathbf{p}\neq\mathbf{0}} a^\dagger_\mathbf{p} a_\mathbf{p}$.] First of all, note that $0 \geq \inf_{1\leq n\leq N} E^n_\ell$, so we can restrict our attention to the values of n such that $E^n_\ell \leq 0$. As proved in the next lemma, such values of n cannot be too small, namely they all satisfy $n \geq c\rho\ell^3$ for a suitable constant c. We can thus assume, without loss of generality, that $n \geq c\rho\ell^3$ in the following.

Lemma 3.3 *If ℓ/R and t^{-1} are large enough, then $H^n_\ell \geq 0$ if $n \leq \rho\ell^3/4$.*

Proof From the definition of H^n_ℓ we see immediately that

$$H^n_\ell \geq \frac{\gamma a_0 R}{R_0^4}\left[-\rho\sum_{j=1}^n \int d\mathbf{y} w_R(\mathbf{x}_i,\mathbf{y}) + \frac{\rho^2}{2}\iint d\mathbf{x} d\mathbf{y} w_R(\mathbf{x},\mathbf{y})\right]$$
$$\geq 2\pi\frac{\gamma a_0 R^4}{R_0^4}\left(-4n\rho + \rho^2\ell^3\right), \tag{3.19}$$

where we used that $\sup_\mathbf{x}\int w_R(\mathbf{x},\mathbf{y})\,d\mathbf{y} \leq 8\pi R^3$ and that, for ℓ/R and t^{-1} large enough, $\iint d\mathbf{x}d\mathbf{y}w_R(\mathbf{x},\mathbf{y}) \geq 4\pi R^3\ell^3$. This proves the lemma. □

A similar argument allows us to get a preliminary bound on the average number of particles outside the condensate $\langle\hat{n}_+\rangle$.

Lemma 3.4 *If t and $(R_0 - R)R_0^{-1}$ are small enough, then for any state such that $\langle H^n_\ell\rangle \leq 0$, the expectation of the number of excited particles satisfies $\langle\hat{n}_+\rangle \leq \mathrm{const}\, n a_0 \ell^2 R_0^{-3}$.*

Proof Using the fact that the potential $e^{-|\mathbf{x}|/R}$ is positive definite, we obtain

$$H^n_\ell \geq -\sum_{i=1}^n \Delta^{(j)}_\ell - \frac{\gamma a_0 R}{2R_0^4}\sum_{i=1}^n w_R(\mathbf{x}_i,\mathbf{x}_i). \tag{3.20}$$

The claim of the lemma follows by using $\langle -\sum_{i=1}^n \Delta^{(j)}_\ell\rangle \geq \langle\hat{n}_+\rangle\pi^2/\ell^2$ and the fact that $w_R(\mathbf{x},\mathbf{x}) \leq 1$. □

Of course, in order for the bound in Lemma 3.4 to be useful, it must be $a_0\ell^2 R_0^{-3} \ll 1$. In the following we shall impose this condition by requiring that, in terms of the scaling exponents introduced in the previous section, $2b + 3d < 1/2$. We shall define $\nu_0 = 1/2 - 2b - 3d$, so that our preliminary a priori bound reads $\langle\hat{n}_+\rangle/n \leq Y^{\nu_0}$.

3.4 Bound on the Unimportant Part of the Hamiltonian

Motivated by Bogoliubov's computation of the ground state energy, we would like to be able to neglect in H^n_ℓ all terms but those containing precisely two $a^\#_\mathbf{p}$, with $\mathbf{p}\neq\mathbf{0}$. Let $\hat{n}_\mathbf{0} = a^\dagger_\mathbf{0} a_\mathbf{0}$ and let us rewrite (3.17) in the form

$$H^n_\ell = \sum_\mathbf{p} \mathbf{p}^2 a^\dagger_\mathbf{p} a_\mathbf{p} + \frac{\gamma a_0 R}{2R_0^4}\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}}(a^\dagger_\mathbf{p} a^\dagger_\mathbf{q} a_\mathbf{0} a_\mathbf{0} + 2a^\dagger_\mathbf{p} a^\dagger_\mathbf{0} a_\mathbf{0} a_\mathbf{q} + a^\dagger_\mathbf{0} a^\dagger_\mathbf{0} a_\mathbf{p} a_\mathbf{q})$$
$$+ \frac{\gamma a_0 R}{2R_0^4}\Big[\hat{w}_{\mathbf{00},\mathbf{00}}\left[(\hat{n}_0 - \rho\ell^3)^2 - \hat{n}_0\right]$$

$$+2\sum_{\mathbf{p}\neq\mathbf{0}}\hat{w}_{\mathbf{p0},\mathbf{00}}\big[(\hat{n}_0-\rho\ell^3)a^\dagger_{\mathbf{p}}a_{\mathbf{0}}+a^\dagger_{\mathbf{0}}a_{\mathbf{p}}(\hat{n}_0-\rho\ell^3)\big]$$
$$+2\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}}\hat{w}_{\mathbf{p0},\mathbf{q0}}a^\dagger_{\mathbf{p}}a_{\mathbf{q}}(\hat{n}_0-\rho\ell^3)+2\sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu}\neq\mathbf{0}}\hat{w}_{\mathbf{pq},\boldsymbol{\mu}\mathbf{0}}(a^\dagger_{\mathbf{p}}a^\dagger_{\mathbf{q}}a_{\boldsymbol{\mu}}a_{\mathbf{0}}+a^\dagger_{\mathbf{0}}a^\dagger_{\boldsymbol{\mu}}a_{\mathbf{q}}a_{\mathbf{p}})$$
$$+\sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu},\boldsymbol{\nu}\neq\mathbf{0}}\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}}a^\dagger_{\mathbf{p}}a^\dagger_{\mathbf{q}}a_{\boldsymbol{\mu}}a_{\boldsymbol{\nu}}\Bigg]. \tag{3.21}$$

We would like to show that all terms but those in the first line are negligible. Let us then estimate all these contributions in terms of $\hat{n}_+$ and $n-\rho\ell^3$. We shall use, without proof, a number of lemmas from [7]. Note that from now on we shall always assume valid the conditions discussed in Sect. 3.2 above. Note also that $\hat{n}_0=n-\hat{n}_+$ and $|\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}}|\leq \text{const}\,R^3/\ell^3$.

1. The first term in the second line of (3.21) satisfies

$$\frac{\gamma a_0 R}{2R_0^4}\hat{w}_{\mathbf{00},\mathbf{00}}\left[(\hat{n}_0-\rho\ell^3)^2-\hat{n}_0\right]\geq \text{const}\,\frac{a_0}{\ell^3}(\hat{n}_0-\rho\ell^3)^2-\text{const}\,\frac{na_0}{\ell^3} \tag{3.22}$$

and, for any $\varepsilon>0$

$$\frac{\gamma a_0 R}{2R_0^4}\hat{w}_{\mathbf{00},\mathbf{00}}\left[(\hat{n}_0-\rho\ell^3)^2-\hat{n}_0\right]$$
$$\geq\frac{\gamma a_0 R}{2R_0^4}\hat{w}_{\mathbf{00},\mathbf{00}}(1-\varepsilon)(n-\rho\ell^3)^2-\text{const}\,\frac{a_0}{\ell^3}\frac{\hat{n}_+^2}{\varepsilon}-\text{const}\,\frac{a_0 n}{\ell^3}. \tag{3.23}$$

2. By Lemma 5.5 of [7], the second term in the second line of (3.21) satisfies for any $\varepsilon>0$

$$\frac{\gamma a_0 R}{R_0^4}\sum_{\mathbf{p}\neq\mathbf{0}}\hat{w}_{\mathbf{p0},\mathbf{00}}\big[(\hat{n}_0-\rho\ell^3)a^\dagger_{\mathbf{p}}a_{\mathbf{0}}+a^\dagger_{\mathbf{0}}a_{\mathbf{p}}(\hat{n}_0-\rho\ell^3)\big]$$
$$\geq-\text{const}\,\frac{\hat{n}_+}{\varepsilon}\frac{na_0}{\ell^3}-\text{const}\,\varepsilon\frac{a_0}{\ell^3}(\hat{n}_0-\rho\ell^3)^2-\text{const}\,\varepsilon\frac{a_0}{\ell^3} \tag{3.24}$$

and

$$\frac{\gamma a_0 R}{R_0^4}\sum_{\mathbf{p}\neq\mathbf{0}}\hat{w}_{\mathbf{p0},\mathbf{00}}\big[(\hat{n}_0-\rho\ell^3)a^\dagger_{\mathbf{p}}a_{\mathbf{0}}+a^\dagger_{\mathbf{0}}a_{\mathbf{p}}(\hat{n}_0-\rho\ell^3)\big]$$
$$\geq\frac{\gamma a_0 R}{R_0^4}\sum_{\mathbf{p}\neq\mathbf{0}}\hat{w}_{\mathbf{p0},\mathbf{00}}\big[(n-\rho\ell^3)a^\dagger_{\mathbf{p}}a_{\mathbf{0}}+a^\dagger_{\mathbf{0}}a_{\mathbf{p}}(n-\rho\ell^3)\big]-\text{const}\,\varepsilon\hat{n}_+\frac{a_0 n}{\ell^3}$$
$$-\text{const}\,\frac{\hat{n}_+^2}{\varepsilon}\frac{a_0}{\ell^3}. \tag{3.25}$$

3. By Lemma 5.3 of [7] the first term in the third line of (3.21) satisfies

$$\frac{\gamma a_0 R}{R_0^4}\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}}\hat{w}_{\mathbf{p0},\mathbf{q0}}a^\dagger_{\mathbf{p}}a_{\mathbf{q}}(\hat{n}_0-\rho\ell^3)\geq-\text{const}\,\frac{a_0}{\ell^3}[\rho\ell^3-n]_+\hat{n}_+-\text{const}\,\frac{a_0\hat{n}_+^2}{\ell^3} \tag{3.26}$$

where $[t]_+=\max\{t,0\}$.

4. By Lemma 5.6 of [7] and its proof, the second term in the third line of (3.21) satisfies for any $\varepsilon > 0$

$$\frac{\gamma a_0 R}{R_0^4} \sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\boldsymbol{\mu}\mathbf{0}}(a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\mathbf{0}} + a_{\mathbf{0}}^\dagger a_{\boldsymbol{\mu}}^\dagger a_{\mathbf{q}} a_{\mathbf{p}})$$
$$\geq -\text{const}\, \varepsilon \frac{a_0 n}{\ell^3}\hat{n}_+ - \text{const}\,\frac{1}{\varepsilon}\frac{a_0 \hat{n}_+}{R^3} - \frac{1}{\varepsilon}\frac{\gamma a_0 R}{R_0^4} \sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu},\boldsymbol{\nu}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\boldsymbol{\nu}}. \quad (3.27)$$

5. The term in the fourth line of (3.21) satisfies

$$0 \leq \frac{\gamma a_0 R}{2R_0^4} \sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu},\boldsymbol{\nu}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\boldsymbol{\nu}} \leq \text{const}\,\frac{a_0 \hat{n}_+^2}{R^3}. \quad (3.28)$$

This follows immediately from the fact that $w_R(\mathbf{x},\mathbf{y}) \leq 1$.

Remark According to Bogoliubov's theory we expect that in the ground state $\langle \hat{n}_+ \rangle \sim n\sqrt{\rho a_0^3}$. From the upper bound in (3.28) we thus expect that the contribution to the ground state energy from the quartic term $\frac{\gamma a_0 R}{2R_0^4}\sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu},\boldsymbol{\nu}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\boldsymbol{\nu}}$ is at most $\sim n^2 \rho a_0 \frac{a_0^3}{R^3}$. In order to show that Bogoliubov theory is asymptotically correct up to terms of order $n\rho a_0\sqrt{\rho a_0^3}$ we shall require such a bound to be much smaller than $n\rho a_0\sqrt{\rho a_0^3}$. For $n \sim \rho\ell^3$ and in terms of the scaling exponents introduced above, this implies $Y^{1/2-3b-3d} \ll 1$, that is $3b + 3d < 1/2$. In the following we shall assume this condition valid. It will be convenient to summarize here all the requirement we asked for so far on the scaling exponents introduced in Sect. 3.2:

$$2b - d > \tau > d \quad \text{and} \quad \frac{1}{6} > b + d > \tau. \quad (3.29)$$

From now on we shall always assume that these relations are valid and that Y is small enough.

3.5 The Quadratic Hamiltonian

In this section we consider the main part of the Hamiltonian. This is the "quadratic" Hamiltonian considered by Bogoliubov. It consists of the kinetic energy and all the terms with the coefficients $\hat{w}_{\mathbf{pq},\mathbf{00}}$, $\hat{w}_{\mathbf{00},\mathbf{pq}}$ $\hat{w}_{\mathbf{p0},\mathbf{0q}}$, and $\hat{w}_{\mathbf{0p},\mathbf{q0}}$ with $\mathbf{p},\mathbf{q}\neq\mathbf{0}$, i.e.,

$$H_B = \sum_{\mathbf{p}} \mathbf{p}^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{\gamma a_0 R}{2R_0^4}\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}}(a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{0}} a_{\mathbf{0}} + 2a_{\mathbf{p}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{0}} a_{\mathbf{q}} + a_{\mathbf{0}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}}). \quad (3.30)$$

In order to compute all the bounds we find it necessary to include the first term in the second line of (3.25) into the "quadratic" Hamiltonian. We therefore define

$$H_Q = \sum_{\mathbf{p}} \mathbf{p}^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{\gamma a_0 R}{R_0^4}\sum_{\mathbf{p}\neq\mathbf{0}} \hat{w}_{\mathbf{p0},\mathbf{00}}\big[(n-\rho\ell^3)a_{\mathbf{p}}^\dagger a_{\mathbf{0}} + a_{\mathbf{0}}^\dagger a_{\mathbf{p}}(n-\rho\ell^3)\big]$$
$$+ \frac{\gamma a_0 R}{2R_0^4}\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}}(a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{0}} a_{\mathbf{0}} + 2a_{\mathbf{p}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{0}} a_{\mathbf{q}} + a_{\mathbf{0}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}}). \quad (3.31)$$

Note that $H_B = H_Q$ in the neutral case $n = \rho\ell^3$. Our goal is to give a lower bound on the ground state energy of the Hamiltonian H_Q.

For any $\mathbf{k} \in \mathbb{R}^3$ denote $\chi_{\ell,\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\mathbf{x}}\chi(\mathbf{x}/\ell)$ and define the operators

$$b_{\mathbf{k}}^\dagger = \sum_{\mathbf{p}\neq\mathbf{0}} (\phi_{\mathbf{p}}, \chi_{\ell,\mathbf{k}}) a_{\mathbf{p}}^\dagger a_{\mathbf{0}} \quad \text{and} \quad b_{\mathbf{k}} = \sum_{\mathbf{p}\neq\mathbf{0}} (\chi_{\ell,\mathbf{k}}, \phi_{\mathbf{p}}) a_{\mathbf{0}}^\dagger a_{\mathbf{p}}. \tag{3.32}$$

Note that they satisfy the commutation relations

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] = \hat{n}_{\mathbf{0}}(\chi_{\ell,\mathbf{k}}, \chi_{\ell,\mathbf{k}'}) - \sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} (\chi_{\ell,\mathbf{k}}, \phi_{\mathbf{p}})(\phi_{\mathbf{q}}, \chi_{\ell,\mathbf{k}'}) a_{\mathbf{q}}^\dagger a_{\mathbf{p}} - \hat{n}_{\mathbf{0}}(\chi_{\ell,\mathbf{k}}, \phi_{\mathbf{0}})(\phi_{\mathbf{0}}, \chi_{\ell,\mathbf{k}'}). \tag{3.33}$$

Using Lemma 6.2 of [7] we find that

$$\left\langle \sum_{\mathbf{p}} |\mathbf{p}|^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} \right\rangle \geq (1 - C't)^2 n^{-1} \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \frac{|\mathbf{k}|^4}{|\mathbf{k}|^2 + (\ell t^3)^{-2}} \langle b_{\mathbf{k}}^\dagger b_{\mathbf{k}} \rangle \tag{3.34}$$

for a suitable constant C' and for all states with particle number equal to n.

Concerning the potential energy terms, note that we may write

$$w_R(\mathbf{x}, \mathbf{y}) = \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \hat{V}_R(\mathbf{k}) \chi_{\ell,\mathbf{k}}(\mathbf{x}) \chi_{\ell,\mathbf{k}}^*(\mathbf{y}), \tag{3.35}$$

where $\hat{V}_R(\mathbf{k}) = 8\pi R^3[1 + (\mathbf{k}R)^2]^{-2}$. The last two sums in the Hamiltonian (3.31) can therefore be written as

$$\begin{aligned}&\frac{\gamma a_0 R}{R_0^4 \ell^3} \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \hat{V}_R(\mathbf{k}) \Big[(n - \rho\ell^3)\ell^{3/2} (\hat{\chi}(\mathbf{k}\ell) b_{\mathbf{k}}^\dagger + \hat{\chi}^*(\mathbf{k}\ell) b_{\mathbf{k}}) \\ &\quad + \frac{1}{2}(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{\mathbf{k}} b_{-\mathbf{k}}) \Big] - \frac{\gamma a_0 R}{R_0^4} \sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}.\end{aligned} \tag{3.36}$$

Thus, we have for states with particle number equal to n that

$$\langle H_Q \rangle \geq \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \langle h_Q(\mathbf{k}) \rangle - \frac{\gamma a_0 R}{R_0^4} \sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}} \langle a_{\mathbf{p}}^\dagger a_{\mathbf{q}} \rangle, \tag{3.37}$$

where

$$\begin{aligned}h_Q(\mathbf{k}) &= \frac{(1 - C't)^2}{2n} \frac{|\mathbf{k}|^4}{|\mathbf{k}|^2 + (\ell t^3)^{-2}} (b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}) \\ &\quad + \frac{\gamma a_0 R}{2R_0^4 \ell^3} \hat{V}_R(\mathbf{k}) \big[(n - \rho\ell^3)\ell^{3/2} \big(\hat{\chi}(\mathbf{k}\ell)(b_{\mathbf{k}}^\dagger + b_{-\mathbf{k}}) + \hat{\chi}^*(\mathbf{k}\ell)(b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger) \big) \\ &\quad + b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}} + b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{\mathbf{k}} b_{-\mathbf{k}} \big].\end{aligned} \tag{3.38}$$

In order to give a lower bound on $h_Q(\mathbf{k})$, we can use Bogoliubov's method, in form of Theorem 6.3 of [7]. This theorem states that, for arbitrary constants $\mathcal{A} \geq \mathcal{B} > 0$ and $\kappa \in \mathbb{C}$, the inequality

$$\mathcal{A}(b_{\mathbf{k}}^\dagger b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger b_{-\mathbf{k}}) + \mathcal{B}(b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger + b_{\mathbf{k}} b_{-\mathbf{k}}) + \kappa(b_{\mathbf{k}}^\dagger + b_{-\mathbf{k}}) + \kappa^*(b_{\mathbf{k}} + b_{-\mathbf{k}}^\dagger)$$
$$\geq -\frac{1}{2}\big(\mathcal{A} - \sqrt{\mathcal{A}^2 - \mathcal{B}^2}\big)([b_{\mathbf{k}}, b_{\mathbf{k}}^\dagger] + [b_{-\mathbf{k}}, b_{-\mathbf{k}}^\dagger]) - \frac{2|\kappa|^2}{\mathcal{A}+\mathcal{B}} \tag{3.39}$$

holds. Note that in our case

$$[b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger] \leq \hat{n}_{\mathbf{0}} \int d\mathbf{x}\, \chi(\mathbf{x}/\ell)^2 \leq n\ell^3. \tag{3.40}$$

With the notation

$$\mathcal{B}_{\mathbf{k}} = \frac{\gamma a_0 R}{2R_0^4 \ell^3} \hat{V}_R(\mathbf{k}),$$
$$\mathcal{A}_{\mathbf{k}} = \frac{(1-C't)^2}{2n} \frac{|\mathbf{k}|^4}{|\mathbf{k}|^2 + (\ell t^3)^{-2}} + \mathcal{B}_{\mathbf{k}}, \tag{3.41}$$
$$\kappa_{\mathbf{k}} = \frac{\gamma a_0 R}{2R_0^4 \ell^{3/2}} \hat{V}_R(\mathbf{k})(n - \rho\ell^3)\hat{\chi}(\mathbf{k}\ell)$$

we thus obtain that on the subspace of n particles

$$h_Q(\mathbf{k}) \geq -n\ell^3\big(\mathcal{A}_{\mathbf{k}} - \sqrt{\mathcal{A}_{\mathbf{k}}^2 - \mathcal{B}_{\mathbf{k}}^2}\big) - \frac{2|\kappa_{\mathbf{k}}|^2}{\mathcal{A}_{\mathbf{k}} + \mathcal{B}_{\mathbf{k}}}. \tag{3.42}$$

Moreover, since

$$\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}} = \int \frac{d\mathbf{x}}{\ell^3} \int d\mathbf{y}\, w_R(\mathbf{x},\mathbf{y}) \Big[\sum_{\mathbf{p}\neq\mathbf{0}} \phi_{\mathbf{p}}(\mathbf{x}) a_{\mathbf{p}}\Big]^\dagger \Big[\sum_{\mathbf{p}\neq\mathbf{0}} \phi_{\mathbf{p}}(\mathbf{y}) a_{\mathbf{p}}\Big]$$
$$\leq \int \frac{d\mathbf{x}}{\ell^3} \int d\mathbf{y}\, w_R(\mathbf{x},\mathbf{y}) \Big[\sum_{\mathbf{p}\neq\mathbf{0}} \phi_{\mathbf{p}}(\mathbf{x}) a_{\mathbf{p}}\Big]^\dagger \Big[\sum_{\mathbf{p}\neq\mathbf{0}} \phi_{\mathbf{p}}(\mathbf{x}) a_{\mathbf{p}}\Big] \leq \frac{8\pi R^3}{\ell^3} \hat{n}_+ \tag{3.43}$$

we have that

$$\frac{\gamma a_0 R}{R_0^4} \sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}} \leq \text{const}\, n \frac{a_0}{\ell^3}. \tag{3.44}$$

Using (3.37), (3.42) and (3.44), we find that, on the subspace with n particles,

$$H_Q \geq -\int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \left\{ n\ell^3\big(\mathcal{A}_{\mathbf{k}} - \sqrt{\mathcal{A}_{\mathbf{k}}^2 - \mathcal{B}_{\mathbf{k}}^2}\big) + \frac{2|\kappa_{\mathbf{k}}|^2}{\mathcal{A}_{\mathbf{k}} + \mathcal{B}_{\mathbf{k}}} \right\} - \text{const}\, n \frac{a_0}{\ell^3}. \tag{3.45}$$

Now, using $\mathcal{A}_{\mathbf{k}} \geq \mathcal{B}_{\mathbf{k}}$ and the definitions of $\mathcal{B}_{\mathbf{k}}, \kappa_{\mathbf{k}}$, we get

$$\int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \frac{2|\kappa_{\mathbf{k}}|^2}{\mathcal{A}_{\mathbf{k}} + \mathcal{B}_{\mathbf{k}}} \leq \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \frac{|\kappa_{\mathbf{k}}|^2}{\mathcal{B}_{\mathbf{k}}}$$
$$= \frac{\gamma a_0 R}{2R_0^4} (n - \rho\ell^3)^2 \int_{\mathbb{R}^3} \frac{d\mathbf{k}}{(2\pi)^3} \hat{V}_R(\mathbf{k}) |\hat{\chi}(\mathbf{k}\ell)|^2$$
$$= \frac{\gamma a_0 R}{2R_0^4} (n - \rho\ell^3)^2 \hat{w}_{\mathbf{00},\mathbf{00}}. \tag{3.46}$$

As a result, on the subspace with n particles,

$$H_Q \geq -nI - \frac{\gamma a_0 R}{2R_0^4}(n - \rho\ell^3)^2 \hat{w}_{\mathbf{00},\mathbf{00}} - \text{const}\, n\frac{a_0}{\ell^3}, \tag{3.47}$$

where

$$\begin{aligned} I &= \frac{1}{2\rho}\int \frac{d\mathbf{k}}{(2\pi)^3}\Big[f(\mathbf{k}) - \sqrt{f(\mathbf{k})^2 - g(\mathbf{k})^2}\Big], \\ f(\mathbf{k}) &= (1 - C't)^2 \frac{\rho\ell^3}{n}\frac{|\mathbf{k}|^4}{|\mathbf{k}|^2 + (\ell t^3)^{-2}} + \frac{\gamma a_0 R\rho}{R_0^4}\hat{V}_R(\mathbf{k}), \\ g(\mathbf{k}) &= \frac{\gamma a_0 R\rho}{R_0^4}\hat{V}_R(\mathbf{k}). \end{aligned} \tag{3.48}$$

Similarly, the Bogoliubov Hamiltonian in (3.30) on the subspace with n particles admits the lower bound

$$H_B \geq -nI - \text{const}\, n\frac{a_0}{\ell^3}. \tag{3.49}$$

Note that $f > g > 0$ implies $f - \sqrt{f^2 - g^2} \leq \min\{g, g^2/(f-g)\}$. Thus clearly I can be bounded as $I \leq (2\pi)^{-3}(2\rho)^{-1}\int d\mathbf{k} g(\mathbf{k}) \leq \text{const}\, a_0 R^{-3}$, so that

$$H_B \geq -\text{const}\, n\frac{a_0}{R^3}. \tag{3.50}$$

Moreover, if $n \leq C\rho\ell^3$, we find

$$\begin{aligned} I &\leq \frac{1}{2\rho}\left\{\int_{|\mathbf{k}|^2 \leq a_0\rho}\frac{d\mathbf{k}}{(2\pi)^3}g(\mathbf{k}) + \int_{|\mathbf{k}|^2 \geq a_0\rho}\frac{d\mathbf{k}}{(2\pi)^3}\frac{g(\mathbf{k})^2}{f(\mathbf{k}) - g(\mathbf{k})}\right\} \\ &\leq \text{const}\left\{\rho a_0\sqrt{\rho a_0^3} + \rho a_0^2\int_{\sqrt{\rho a_0}}^{\infty} dk\frac{1}{[(kR)^2 + 1]^4}\left(1 + (k\ell t^3)^{-2}\right)\right\} \\ &\leq \text{const}\,\rho a_0\left\{\sqrt{\rho a_0^3} + \frac{a_0}{R}\left[1 + \frac{1}{\sqrt{\rho a_0}R}\left(\frac{R}{\ell t^3}\right)^2\right]\right\}. \end{aligned} \tag{3.51}$$

If the scaling exponents satisfy

$$2b + d - 6\tau > 0, \tag{3.52}$$

then the last expression in (3.51) can be bounded from above by $\text{const}\,\rho a_0\frac{a_0}{R}$. Hence, if $n \leq C\rho\ell^2$ and $2b + d - 6\tau > 0$,

$$H_B \geq -\text{const}\, n\rho a_0\frac{a_0}{R}. \tag{3.53}$$

3.6 Improved Bounds on n

Using the bounds derived in the previous sections, we shall now get an improved bound on n, which implies that for states with $\langle H_\ell^n\rangle \leq 0$, n cannot deviate too much from $\rho\ell^3$. In order to bound (3.21) from below, we use (3.22), (3.24), (3.26), (3.27) and (3.50) [note that we shall use (3.27) with ε replaced by ε^{-1}]. The result is that, for some positive constants c and C, we have

$$H_\ell^n \geq (c - C\varepsilon)\frac{a_0}{\ell^3}(\hat{n}_0 - \rho\ell^3)^2 + (1 - C\varepsilon)\frac{\gamma a_0 R}{2R_0^4}\sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu},\boldsymbol{\nu}\neq 0}\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\boldsymbol{\nu}}$$
$$- C\left\{\frac{na_0}{\ell^3} + \frac{\hat{n}_+}{\varepsilon}\frac{na_0}{\ell^3} + \varepsilon\frac{a_0}{\ell^3} + \frac{a_0}{\ell^3}\rho\ell^3\hat{n}_+ + \frac{a_0\hat{n}_+^2}{\ell^3} + \varepsilon\frac{a_0\hat{n}_+}{R^3} + n\frac{a_0}{R^3}\right\} \quad (3.54)$$

for some $\varepsilon > 0$. Choosing $\varepsilon = \min\{1, c\}/(2C)$, using $\hat{n}_+ \leq n$, $\sum_{\mathbf{p},\mathbf{q},\boldsymbol{\mu},\boldsymbol{\nu}\neq 0}\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}} a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\boldsymbol{\mu}} a_{\boldsymbol{\nu}} \geq 0$ and recalling that, by Lemma 3.3, $n \leq \rho\ell^3/4$ implies $H_\ell^n \geq 0$, we have, for some new constants c' and C' and for any state with $\langle H_\ell^n\rangle \leq 0$,

$$0 \geq \langle H_\ell^n\rangle \geq c'\frac{a_0}{\ell^3}\langle(\hat{n}_0 - \rho\ell^3)^2\rangle - C'\frac{a_0}{\ell^3}\left\{n\langle\hat{n}_+\rangle + \frac{n^2}{\rho R^3}\right\} \quad (3.55)$$

and, therefore,

$$\frac{(n - \rho\ell^3)^2}{n^2} \leq \text{const}\left\{\frac{\langle\hat{n}_+\rangle}{n} + \frac{1}{\rho R^3}\right\}. \quad (3.56)$$

Here, we used $\langle(\hat{n}_0 - \rho\ell^3)^2\rangle \geq (n - \rho\ell^3)^2 - 2n\langle\hat{n}_+\rangle$. Now, let us recall from Sect. 3.3 that, in terms of the scaling exponents b, d, we have $\langle\hat{n}_+\rangle/n \leq Y^{\frac{1}{2}-2b-3d}$, and $(\rho R^3)^{-1} \sim Y^{\frac{1}{2}-3d}$, so that

$$\frac{(n - \rho\ell^3)^2}{n^2} \leq \text{const}\, Y^{\nu_0}, \quad (3.57)$$

where $\nu_0 = 1/2 - 2b - 3d$ as before. Equation (3.57) can be rewritten as

$$\left|n - \rho\ell^3\right| \leq \text{const}\,\rho\ell^3 Y^{\nu_0/2}. \quad (3.58)$$

In order to get the bounds above we sacrificed all the kinetic energy in (3.21). Of course this is not necessary: we can decide to sacrifice only half of it and we would still get the same bounds, only with different constants. If we proceed in this way we see that for any n-particle state such that $\langle H_\ell^n\rangle \leq 0$,

$$\sum_{\mathbf{p}}|\mathbf{p}|^2\langle a_{\mathbf{p}}^\dagger a_{\mathbf{p}}\rangle \leq \text{const}\, n\rho a_0 Y^{\nu_0}. \quad (3.59)$$

3.7 Localization of n_+

The idea now is to use the improved bound on n together with the bounds in previous sections in order to find an improved bound on the energy of the ground state. In order to do this it is clear from the bounds in Sect. 3.4 that we need to estimate $\langle\hat{n}_+^2\rangle$. Since we have bounded only $\hat{n}_+$ so far, we would like to argue that $\langle\hat{n}_+^2\rangle \approx \langle\hat{n}_+\rangle^2$. In this section we shall discuss how to do this. We shall utilize the following theorem, which is Theorem A.1 of [7]. [The kth supra- (resp. infra-) diagonal of a matrix $\mathcal{A}$ is the submatrix consisting of all elements $a_{i,i+k}$ (resp. $a_{i+k,i}$)].

Theorem 3.1 *Suppose that $\mathcal{A}$ is an $N \times N$ Hermitean matrix and let $\mathcal{A}^k$, with $k = 0, 1, \ldots, N-1$, denote the matrix consisting of the* kth *supra- and infra-diagonal of $\mathcal{A}$. Let $\psi \in \mathbf{C}^N$ be a normalized vector and set $d_k = (\psi, \mathcal{A}^k\psi)$ and $\lambda = (\psi, \mathcal{A}\psi) = \sum_{k=0}^{N-1} d_k$*

(ψ *need not be an eigenvector of* $\mathcal{A}$). *Choose some positive integer* $M \le N$. *Then, with* M *fixed, there is some* $n \in [0, N-M]$ *and some normalized vector* $\phi \in \mathbf{C}^N$ *with the property that* $\phi_j = 0$ *unless* $n+1 \le j \le n+M$ (*i.e.,* ϕ *has length* M) *and such that*

$$(\phi, \mathcal{A}\phi) \le \lambda + \frac{C}{M^2}\sum_{k=1}^{M-1} k^2|d_k| + C\sum_{k=M}^{N-1}|d_k|, \tag{3.60}$$

where $C > 0$ *is a universal constant.* (*Note that the first sum starts with* $k = 1$.)

From this theorem we can get a localization bound on $\hat{n}_+$ in the following way. Consider a normalized n-particle wavefunction Ψ, which we may write as $\Psi = \sum_{m=0}^{n} c_m \Psi_m$, where for all $m = 0, 1, 2, \ldots, n$, Ψ_m is a normalized eigenfunction of $\hat{n}_+$ with eigenvalue m. We now consider the $(n+1)\times(n+1)$ Hermitean matrix $\mathcal{A}$ with matrix elements $\mathcal{A}_{mm'} = (\Psi_m, H_\ell^n \Psi_{m'})$.

We shall use Theorem 3.1 for this matrix and the vector $\psi = (c_0, \ldots, c_n)$. We shall choose M in Theorem 3.1 to be of the order of the upper bound on $\langle \hat{n}_+ \rangle$ derived in Lemma 3.4, e.g., M is the integer part of nY^{ν_0}. Note that, if $n \sim \rho\ell^3$, we have $M \gg 1$. With the notation in Theorem 3.1 we have $\lambda = (\psi, \mathcal{A}\psi) = (\Psi, H_\ell^n \Psi)$. Note also that because of the structure of H_ℓ^n we have, again with the notation from Theorem 3.1, that $d_k = 0$ if $k \ge 3$. We conclude from it that there exists a normalized wavefunction $\widetilde{\Psi}$ with the property that the corresponding $\hat{n}_+$ values belong to an interval of length $M \sim nY^{\nu_0}$ and such that

$$\big(\Psi, H_\ell^n \Psi\big) \ge \big(\widetilde{\Psi}, H_\ell^n \widetilde{\Psi}\big) - \text{const}\,\frac{1}{n^2 Y^{2\nu_0}}(|d_1| + |d_2|). \tag{3.61}$$

We shall now bound d_1 and d_2. We have $d_1 = (\Psi, H_\ell^n(1)\Psi)$, where $H_\ell^n(1)$ is the part of the Hamiltonian H_ℓ^n containing all the terms with the coefficients $\hat{w}_{\mathbf{pq},\boldsymbol{\mu\nu}}$ for which precisely one or three indices are $\mathbf{0}$. These are the terms bounded in (3.24) and (3.27). These estimates are stated as one-sided bounds. It is however clear that they could have been stated as two sided bounds. Using in addition the bound (3.28) and $\hat{n}_+^2 \le n\hat{n}_+$ then, for any $\varepsilon > 0$ and some positive constant C, we get

$$|d_1| \le C\left(\Psi, \left[\frac{\hat{n}_+}{\varepsilon}\frac{na_0}{\ell^3} + \varepsilon\frac{a_0}{\ell^3}(\hat{n}_0 - \rho\ell^3)^2 + \varepsilon\frac{a_0}{\ell^3} + \varepsilon\frac{a_0 n\hat{n}_+}{R^3}\right]\Psi\right). \tag{3.62}$$

If Ψ satisfies $(\Psi, H_\ell^n \Psi) \le 0$, we can use Lemma 3.4 and (3.58) to conclude that

$$|d_1| \le Cn\rho a_0\left(\frac{Y^{\nu_0}}{\varepsilon} + \varepsilon Y^{\nu_0 - 3b - 3d}\right). \tag{3.63}$$

Optimizing over $\varepsilon > 0$ yields the bound

$$|d_1| \le Cn\rho a_0 Y^{\nu_0 - \frac{3}{2}(b+d)} = Cn\rho a_0 Y^{\frac{1}{2} - \frac{7}{2}b - \frac{9}{2}d}. \tag{3.64}$$

For d_2 we obtain

$$\begin{aligned} |d_2| &\le \left(\Psi, \frac{\gamma a_0 R}{2R_0^4}\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}}(a_\mathbf{p}^\dagger a_\mathbf{q}^\dagger a_\mathbf{0} a_\mathbf{0} + a_\mathbf{0}^\dagger a_\mathbf{0}^\dagger a_\mathbf{p} a_\mathbf{q})\Psi\right) \\ &= \left(\Psi, \left[\sum_\mathbf{p} \mathbf{p}^2 a_\mathbf{p}^\dagger a_\mathbf{p} + \frac{\gamma a_0 R}{R_0^4}\sum_{\mathbf{p},\mathbf{q}\neq\mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}} a_\mathbf{p}^\dagger a_\mathbf{0}^\dagger a_\mathbf{0} a_\mathbf{q}\right]\Psi\right) - (\Psi, \widetilde{H}_B \Psi) \end{aligned} \tag{3.65}$$

where

$$\widetilde{H}_B = \sum_{\mathbf{p}} \mathbf{p}^2 a_{\mathbf{p}}^\dagger a_{\mathbf{p}} + \frac{\gamma a_0 R}{2R_0^4} \sum_{\mathbf{p},\mathbf{q}\neq \mathbf{0}} \hat{w}_{\mathbf{pq},\mathbf{00}}(-a_{\mathbf{p}}^\dagger a_{\mathbf{q}}^\dagger a_{\mathbf{0}} a_{\mathbf{0}} + 2a_{\mathbf{p}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{0}} a_{\mathbf{q}} - a_{\mathbf{0}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{p}} a_{\mathbf{q}}) \tag{3.66}$$

is an operator unitarily equivalent to H_B. (It is obtained from it by replacing $a_{\mathbf{p}}^\dagger, a_{\mathbf{p}}$ by $-ia_{\mathbf{p}}^\dagger, ia_{\mathbf{p}}$, respectively.) Of course $\widetilde{H}_B$ satisfies the same lower bound (3.53) as H_B. It is not difficult to see that

$$0 \le \frac{\gamma a_0 R}{R_0^4} \sum_{\mathbf{p},\mathbf{q}\neq 0} \hat{w}_{\mathbf{pq},\mathbf{00}} \langle a_{\mathbf{p}}^\dagger a_{\mathbf{0}}^\dagger a_{\mathbf{0}} a_{\mathbf{q}} \rangle \le \frac{4\pi \gamma a_0}{\ell^3} \frac{R^4}{R_0^4} n \langle \hat{n}_+ \rangle \tag{3.67}$$

(compare with Lemma 5.4 of [7]). If Ψ satisfies $(\Psi, H_\ell^n \Psi) \le 0$ then, using (3.65), (3.67), Lemma 3.4, (3.59) and (3.53), we get:

$$|d_2| \le \text{const}\, n\rho a_0 \left\{ Y^{\nu_0} + \frac{a_0}{R} \right\} \le \text{const}\, n\rho a_0 Y^{\nu_0}. \tag{3.68}$$

Putting together these bounds we find that if $(\Psi, H_\ell^n \Psi) \le 0$ then there exists a normalized wavefunction $\widetilde{\Psi}$ with the property that the corresponding $\hat{n}_+$ values belong to an interval of length $M \sim nY^{\nu_0}$ and such that

$$\begin{aligned} \big(\Psi, H_\ell^n \Psi\big) &\ge \big(\widetilde{\Psi}, H_\ell^n \widetilde{\Psi}\big) - \text{const}\, \frac{\rho a_0}{nY^{2\nu_0}} Y^{\nu_0 - \frac{3}{2}(b+d)} \\ &\ge \big(\widetilde{\Psi}, H_\ell^n \widetilde{\Psi}\big) - Cn\rho a_0 Y^{\mu_0}, \end{aligned} \tag{3.69}$$

where $\mu_0 = -\nu_0 + 1 + \frac{9}{2}b - \frac{3}{2}d = \frac{1}{2} + \frac{13}{2}b + \frac{3}{2}d$. Since $\mu_0 > 1/2$, the error term in the last line is much smaller than $n\rho a_0 \sqrt{\rho a_0^3}$. Without loss of generality, we may assume that $(\widetilde{\Psi}, H_\ell^n \widetilde{\Psi}) \le 0$, in which case Lemma 3.4 implies that $(\widetilde{\Psi}, \hat{n}_+ \widetilde{\Psi}) \le \text{const}\, nY^{\nu_0}$. We also know that the possible $\hat{n}_+$ values of $\widetilde{\Psi}$ range in an interval of length $M \sim nY^{\nu_0}$. This implies that if $(\Psi, H_\ell^n \Psi) \le -Cn\rho a_0 Y^{1/2}$ then the allowed values of $\hat{n}_+$ for $\widetilde{\Psi}$ are less than CnY^{ν_0}, for a suitable constant C. In particular, $\langle \hat{n}_+^2 \rangle \le Cn^2 Y^{2\nu_0}$ in the state $\widetilde{\Psi}$. Hence, as far as the derivation of a lower bound on the ground state energy is concerned, it is not a restriction to assume that $\langle \hat{n}_+^2 \rangle \sim \langle \hat{n}_+ \rangle^2$. This fact will be used in the next section to derive improved lower bounds on the ground state energy.

3.8 Improved Bound on the Ground State Energy

Let Ψ be the ground state of H_ℓ^n. In this section we shall get an improved lower bound on $(\Psi, H_\ell^n \Psi)$ under the assumption that $(\Psi, H_\ell^n \Psi)$ is small enough such that (3.69) implies that $(\widetilde{\Psi}, H_\ell^n \widetilde{\Psi}) \le 0$. Note that if this assumption is violated then the desired bound on the ground state energy would automatically be true. Hence, as discussed at the end of previous section we know that

$$(\Psi, H_\ell^n \Psi) \ge \langle H_\ell^n \rangle - Cn\rho a_0 Y^{\mu_0} \tag{3.70}$$

where the average $\langle \cdot \rangle$ is over an n-particle state with allowed values of $\hat{n}_+$ smaller than CnY^{ν_0}. Using (3.21), (3.23), (3.25), (3.26), (3.27) [this time precisely in the form stated, without replacement of ε by ε^{-1}] and (3.28), we find that

$$\langle H_\ell^n \rangle \geq \langle H_Q \rangle + \frac{\gamma a_0 R}{2R_0^4} \hat{w}_{\mathbf{00},\mathbf{00}} (1-\varepsilon)(n-\rho\ell^3)^2 - C\Bigg[\frac{a_0}{\ell^3}\frac{\langle \hat{n}_+^2\rangle}{\varepsilon} + \frac{a_0 n}{\ell^3} + \varepsilon\langle \hat{n}_+\rangle \frac{a_0 n}{\ell^3}$$

$$+ \frac{a_0}{\ell^3}|n-\rho\ell^3|\langle \hat{n}_+\rangle + \frac{a_0\langle \hat{n}_+^2\rangle}{\ell^3} + \varepsilon\frac{a_0 n}{\ell^3}\langle \hat{n}_+\rangle + \frac{1}{\varepsilon}\frac{a_0\langle \hat{n}_+\rangle}{R^3} + \frac{1}{\varepsilon}\frac{a_0\langle \hat{n}_+^2\rangle}{R^3}\Bigg]. \quad (3.71)$$

Now, if $0 < \varepsilon < 1$, using $n_+ \leq CnY^{\nu_0}$, (3.47), and (3.58), we get from the last inequality that

$$\langle H_\ell^n \rangle \geq -nI - Cn\rho a_0 \Bigg[\varepsilon Y^{\nu_0} + Y^{\frac{3}{2}\nu_0} + \frac{1}{\varepsilon} Y^{2\nu_0 - 3b - 3d}\Bigg]. \quad (3.72)$$

Optimizing over ε yields

$$\langle H_\ell^n \rangle \geq -nI - Cn\rho a_0 Y^{\alpha_1}, \quad (3.73)$$

where $\alpha_1 = \frac{3}{2}\nu_0 - \frac{3}{2}b - \frac{3}{2}d = \frac{3}{4} - \frac{9}{2}b - 6d$. If

$$\frac{3}{4} - \frac{9}{2}b - 6d > \frac{1}{2}, \quad (3.74)$$

the error term $n\rho a_0 Y^{\alpha_1}$ is much smaller than $n\rho a_0 Y^{1/2}$ and, therefore,

$$E_\ell^n \geq -nI - n\rho a_0 o(Y^{1/2}). \quad (3.75)$$

We are left with estimating the constant I defined by (3.48). It is not difficult to see that, under the assumptions made so far on the scaling exponents,

$$I = 4\pi\rho a_0 \left(\frac{a_1}{a_0} - \frac{128}{15\sqrt{\pi}}\sqrt{\rho a_0^3} + o\left(\sqrt{\rho a_0^3}\right)\right). \quad (3.76)$$

The conditions (3.29), (3.52) and (3.74) on the scaling exponents that we required for the proof to work can be summarized into the following conditions:

$$2b + d > 6\tau, \quad \tau > d, \quad \frac{1}{6} > 3b + 4d. \quad (3.77)$$

It is easy to check that if $d < 1/69$ then all these requirements on the scaling exponents can be satisfied.

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