The Ground State Energy of a Dilute Bose Gas*†

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Abstract

According to a formula that was put forward many decades ago the ground state energy per particle of an interacting, dilute Bose gas at density ρ is $2\pi\hbar^2\rho a/m$ to leading order in $\rho a^3 \ll 1$, where a is the scattering length of the interaction potential and m the particle mass. This result, which is important for the theoretical description of current experiments on Bose-Einstein condensation, has recently been established rigorously for the first time. We give here an account of the proof that applies to nonnegative, spherically symmetric potentials decreasing faster than $1/r^3$ at infinity.

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1 Introduction

Recent progress in the trapping and cooling of atoms has made the ground state properties of dilute, interacting Bose gases accessible to experimental study [1], [2]. In the theoretical description of such experiments an old formula for the ground state energy plays an important role. This formula, stated precisely in (1.6) below, is the subject of the present contribution, which is essentially an exposition of the paper [3], incorporating some new results from [4] and [5].

We consider the Hamiltonian for N Bosons of mass m enclosed in a cubic box Λ of side length L and interacting by a spherically symmetric pair potential $v(|\vec{x}_i - \vec{x}_j|)$:

$$H_N = -\mu \sum_{i=1}^{N} \Delta_i + \sum_{1 \le i < j \le N} v(|\vec{x}_i - \vec{x}_j|). \tag{1.1}$$

Here $\vec{x}_i \in \mathbb{R}^3$, $i = 1, \dots, N$ are the positions of the particles, Δ_i the Laplacian with respect to $\vec{x}_i$, and we have denoted $\hbar^2/2m$ by μ for short. (By choosing suitable units μ could, of course, be eliminated, but we want to keep track of the dependence of the energy on Planck's constant and the mass.) The Hamiltonian (1.1) operates on *symmetric* wave functions in $L^2(\Lambda^N, d\vec{x}_1 \cdots d\vec{x}_N)$ as is appropriate for Bosons. The interaction potential will be assumed to be *nonnegative* and to decrease faster than $1/r^3$ at infinity.

We are interested in the ground state energy $E_0(N, L)$ of (1.1) in the *thermodynamic limit* when N and L tend to infinity with the density $\rho = N/L^3$ fixed. The energy per particle in this limit

$$e_0(\rho) = \lim_{L \to \infty} E_0(\rho L^3, L)/(\rho L^3). \tag{1.2}$$

Our results about $e_0(\rho)$ are based on estimates on $E_0(N, L)$ for finite N and L, which are important, e.g., for the considerations of inhomogeneous systems in [4]. To define $E_0(N, L)$ precisely one must specify the boundary conditions. These should not matter for the thermodynamic limit. To be on the safe side we use Neumann boundary conditions for the lower bound, and Dirichlet boundary conditions for the upper bound since these lead, respectively, to the lowest and the highest energies.

For experiments with dilute gases the *low density asymptotics* of $e_0(\rho)$ is of importance. Low density means here that the mean interparticle distance, $\rho^{-1/3}$ is much larger than the *scattering length* a of the potential, defined as

$$a = \lim_{r\to\infty} r - \frac{u_0(r)}{u_0'(r)}, \tag{1.3}$$

where u_0 solves the zero energy scattering equation,

$$-2\mu u_0''(r) + v(r)u_0(r) = 0 \tag{1.4}$$

with $u_0(0) = 0$. (The factor 2 in (1.4) comes from the reduced mass of the two particle problem.) Our main result is a rigorous proof of the formula

$$e_0(\rho) \approx 4\pi\mu\rho a \tag{1.5}$$

for $\rho a^3 \ll 1$, more precisely of

Theorem 1.1 (Low density limit of the ground state energy)

$$\lim_{\rho a^3\to 0} \frac{e_0(\rho)}{4\pi\mu\rho a} = 1. \tag{1.6}$$

This formula is independent of the boundary conditions used for the definition of $e_0(\rho)$.

The genesis of an understanding of $e_0(\rho)$ was the pioneering work [6] of Bogoliubov, and in the 50's and early 60's several derivations of (1.6) were presented [7], [8], even including higher order terms:

$$\frac{e_0(\rho)}{4\pi\mu\rho a} = 1 + \tfrac{128}{15\sqrt{\pi}}(\rho a^3)^{1/2} + 8\left(\tfrac{4\pi}{3} - \sqrt{3}\right)(\rho a^3)\log(\rho a^3) + O(\rho a^3) \tag{1.7}$$

These early developments are reviewed in [9]. They all rely on some special assumptions about the ground state that have never been proved, or on the selection of special terms from a perturbation series which likely diverges. The only rigorous estimates of this period were established by Dyson, who derived the following bounds in 1957 for a gas of hard spheres [10]:

$$\frac{1}{10\sqrt{2}} \le \frac{e_0(\rho)}{4\pi\mu\rho a} \le \frac{1+2Y^{1/3}}{(1-Y^{1/3})^2} \tag{1.8}$$

with $Y = 4\pi\rho a^3/3$. While the upper bound has the asymptotically correct form, the lower bound is off the mark by a factor of about 1/14. But for about 40 years this was the best lower bound available!

Since (1.6) is a basic result about the Bose gas it is clearly important to derive it rigorously and in reasonable generality, in particular for more general cases than hard spheres. The question immediately arises for which interaction potentials one may expect it to be true. A notable fact is that it *not true for all* v with $a > 0$, since there are two body potentials with positive scattering length that allow many body bound states [11]. Our proof, presented in the sequel, works for nonnegative v, but we conjecture that (1.6) holds if $a > 0$ and v has no N-body bound states for any N. The lower bound is, of course, the hardest part, but the upper bound is not altogether trivial either.

Before we start with the estimates a simple computation and some heuristics may be helpful to make (1.6) plausible and motivate the formal proofs.

With u_0 the scattering solution and $f_0(r) = u_0(r)/r$, partial integration gives

$$\begin{aligned}\int_{|\vec{x}|\leq R} \{2\mu|\nabla f_0|^2 + v|f_0|^2\} d\vec{x} &= 4\pi \int_0^R \{2\mu[u_0'(r) - (u_0(r)/r)]^2 + v(r)|u_0(r)|^2\} dr \\ &= 8\pi\mu a |u_0(R)|^2/R^2 \to 8\pi\mu a \quad \text{for } R \to \infty, \end{aligned} \tag{1.9}$$

if u_0 is normalized so that $f_0(R) \to 1$ as $R \to \infty$. Moreover, for positive interaction potentials the scattering solution minimizes the quadratic form in (1.9) for each R with $u_0(0) = 0$ and $u_0(R)$ fixed as boundary conditions. Hence the energy $E_0(2, L)$ of two particles in a large box, i.e., $L \gg a$, is approximately $8\pi\mu a/L^3$. If the gas is sufficiently dilute it is not unreasonable to expect that the energy is essentially a sum of all such two particle contributions. Since there are $N(N-1)/2$ pairs, we are thus lead to $E_0(N, L) \approx 4\pi\mu a N(N-1)/L^3$, which gives (1.6) in the thermodynamic limit.

This simple heuristics is far from a rigorous proof, however, especially for the lower bound. In fact, it is rather remarkable that the same asymptotic formula holds both for 'soft' interaction potentials, where perturbation theory can be expected to be a good approximation, and potentials like hard spheres where this is not so. In the former case the ground state is approximately the constant function and the energy is *mostly potential*: According to perturbation theory $E_0(N, L) \approx N(N-1)/(2L^3) \int v(|\vec{x}|) d\vec{x}$. In particular it is *independent of* μ, i.e. of Planck's constant and mass. Since, however,

$\int v(|\vec{x}|)d\vec{x}$ is the first Born approximation to $8\pi\mu a$ (note that a depends on μ!), this is not in conflict with (1.6). For 'hard' potentials on the other hand, the ground state is *highly correlated*, i.e., it is far from being a product of single particle states. The energy is here *mostly kinetic*, because the wave function is very small where the potential is large. These two quite different regimes, the potential energy dominated one and the kinetic energy dominated one, cannot be distinguished by the low density asymptotics of the energy. Whether they behave differently with respect to other phenomena, e.g., Bose-Einstein condensation, is not known at present.

Bogolubov's analysis [6] presupposes the existence of Bose-Einstein condensation. Nevertheless, it is correct (for the energy) for the one-dimensional delta-function Bose gas [12], despite the fact that there is (presumably) no condensation in that case. It turns out that BE condensation is not really needed in order to understand the energy. As we shall see, 'global' condensation can be replaced by a 'local' condensation on boxes whose size is independent of L. It is this crucial understanding that enables us to prove Theorem 1.1 without having to decide about BE condensation.

An important idea of Dyson was to transform the hard sphere potential into a soft potential at the cost of sacrificing the kinetic energy, i.e., effectively to move from one regime to the other. We shall make use of this idea in our proof of the lower bound below. But first we discuss the simpler upper bound, which relies on other ideas from Dyson's beautiful paper [10].

2 Upper bound

The following generalization of Dyson's upper bound holds [4], [5]:

Theorem 2.1 (Upper bound) *Define* $\rho_1 = (N-1)/L^3$ *and* $b = (4\pi\rho_1/3)^{-1/3}$. *For nonnegative potentials* v, *and* $b > a$ *the ground state energy of (1.1) with periodic boundary conditions satisfies*

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \frac{a}{b} + \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1-\frac{a}{b}\right)^8}. \tag{2.1}$$

For Dirichlet boundary conditions the estimate holds with $(\text{const.})/L^2$ *added to the right side. Thus in the thermodynamic limit and for all boundary* *conditions*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \leq \frac{1 - Y^{1/3} + Y^{2/3} - \frac{1}{2}Y}{(1 - Y^{1/3})^8}. \tag{2.2}$$

provided $Y = 4\pi\rho a^3/3 < 1$.

Remark. The bound (2.1) holds for potentials with infinite range, provided $b > a$. For potentials of finite range R_0 it can be improved for $b > R_0$ to

$$E_0(N,L)/N \leq 4\pi\mu\rho_1 a \frac{1 - \left(\frac{a}{b}\right)^2 + \frac{1}{2}\left(\frac{a}{b}\right)^3}{\left(1 - \frac{a}{b}\right)^4}. \tag{2.3}$$

Proof. We first remark that the expectation value of (1.1) with any trial wave function gives an upper bound to the bosonic ground state energy, even if the trial function is not symmetric under permutations of the variables. The reason is that an absolute ground state of the elliptic differential operator (1.1) (i.e. a ground state without symmetry requirement) is a nonnegative function which can be be symmetrized without changing the energy because (1.1) is symmetric under permutations. In other words, the absolute ground state energy is the same as the bosonic ground state energy.

Following [10] we choose a trial function of the following form

$$\Psi(x_1, \ldots, x_N) = F_1(x_1) \cdot F_2(x_1, x_2) \cdots F_N(x_1, \ldots, x_n). \tag{2.4}$$

More specifically, $F_1 \equiv 1$ and F_i depends only on the distance of x_i to its nearest neighbor among the the points $x_1, \ldots, x_{i-1}$ (taking the periodic boundary into account):

$$F_i(x_1, \ldots, x_i) = f(t_i), \quad t_i = \min\left(|x_i - x_j|, j = 1, \ldots, i-1\right), \tag{2.5}$$

with a function f satisfying

$$0 \leq f \leq 1, \quad f' \geq 0. \tag{2.6}$$

The intuition behind the ansatz (2.4) is that the particles are inserted into the system one at the time, taking into account the particles previously inserted. While such a wave function cannot reproduce all correlations present in the true ground state, it turns out to capture the leading term in the energy for dilute gases. The form (2.5) is computationally easier to handle than an ansatz of the type $\prod_{i<j} f(|x_i - x_j|)$, which might appear more natural in view of the heuristic remarks at the end of the last section.

The function f is chosen to be

$$f(r) = \begin{cases} f_0(r)/f_0(b) & \text{for } 0 \le r \le b, \\ 1 & \text{for } r > b, \end{cases} \tag{2.7}$$

with $f_0(r) = u_0(r)/r$. The estimates (2.1) and (2.3) are obtained by somewhat lengthy computations similar as in [10], but making use of (1.9). For details we refer to [4] and [5].

A test wave function with Dirichlet boundary condition may be obtained by localizing the wave function (2.4) on the length scale L. The energy cost per particle for this is (const.)$/L^2$. □

3 Lower bound

To get an idea why the lower bound for the bosonic ground state energy of (1.1) is not easy to obtain let us consider the relevant length scales of the problem. These are

- The scattering length a.
- The mean particle distance $\rho^{-1/3}$.
- The 'uncertainty principle length' ℓ_c, defined by $\mu\ell_c^{-2} = e_0(\rho)$, i.e., $\ell_c \sim (\rho a)^{-1/2}$.

The length ℓ_c is sometimes called 'correlation length' or 'healing length'. The name 'uncertainty principle length' is justified by the fact that this is the shortest length scale on which the bosons can be localized without raising the energy per particle above e_0, according to the uncertainty principle. For dilute gases $\rho a^3 \ll 1$ and hence

$$a \ll \rho^{-1/3} \ll (\rho a^3)^{-1/6} \rho^{-1/3} \sim \ell_c. \tag{3.1}$$

Bosons in their ground state are therefore 'smeared out' over distances large compared to the mean particle distance and their individuality is entirely lost. Fermions, on the other hand, prefer to sit in private rooms, i.e., ℓ_c can be comparable to $\rho^{-1/3}$. In this respect the quantum nature of Bosons is much more pronounced than for Fermions. The three different length scales for Bosons will play a role in the proof below.

Our lower bound for $e_0(\rho)$ is as follows.

Theorem 3.1 (Lower bound in the thermodynamic limit) *For a positive potential v with finite range and Y small enough*

$$\frac{e_0(\rho)}{4\pi\mu\rho a} \geq (1 - C\,Y^{1/17}) \tag{3.2}$$

with C a constant. If v does not have finite range, but decreases at least as fast as $1/r^{3+\varepsilon}$ at infinity with some $\varepsilon > 0$, then an analogous bound to (3.2) holds, but with C replaced by another constant and 1/17 by another exponent, both of which may depend on ε.

It should be noted right away that the error term $-C\,Y^{1/17}$ in (3.2) is of no fundamental significance and is not believed to reflect the true state of affairs. Presumably, it does not even have the right sign. We mention in passing that C can be taken to be 8.9 [5].

As mentioned in the Introduction a lower bound on $E_0(N,L)$ for finite N and L is of importance for applications to inhomogeneous gases, and in fact we derive (3.2) from such a bound. We state it in the following way:

Theorem 3.2 (Lower bound in a finite box) *For a positive potential v with finite range there is a $\delta > 0$ such that the the ground state energy of (1.1) with Neumann conditions satisfies*

$$E_0(N,L)/N \geq 4\pi\mu\rho a \left(1 - C\,Y^{1/17}\right) \tag{3.3}$$

for all N and L with $Y < \delta$ and $L/a > C'Y^{-6/17}$. Here C and C' are constants, independent of N and L. (Note that the condition on L/a requires in particular that N must be large enough, $N > (\mathrm{const.})Y^{-1/17}$.) As in Theorem 3.1 such a bound, but possibly with other constants and another exponent for Y, holds also for potentials v of infinite range decreasing faster than $1/r^3$ at infinity.

The first step in the proof of (3.2) is a generalization of a lemma of Dyson, which allows us to replace v by a 'soft' potential, at the cost of sacrificing kinetic energy and increasing the effective range.

Lemma 3.3 *Let $v(r) \geq 0$ with finite range R_0. Let $U(r) \geq 0$ be any function satisfying $\int U(r)r^2dr \leq 1$ and $U(r) = 0$ for $r < R_0$. Let $\mathcal{B} \subset \mathbf{R}^3$ be star shaped with respect to 0 (e.g. convex with $0 \in \mathcal{B}$). Then for all differentiable functions ψ*

$$\int_{\mathcal{B}} \left[\mu|\nabla\psi|^2 + \tfrac{1}{2}v|\psi|^2\right] \geq \mu a \int_{\mathcal{B}} U|\psi|^2. \tag{3.4}$$

Proof. Actually, (3.4) holds with $\mu|\nabla\phi(\vec{x})|^2$ replaced by the (smaller) radial kinetic energy, $\mu|\partial\phi(\vec{x})/\partial r|^2$, and it suffices to prove the analog of (3.4) for the integral along each radial line with fixed angular variables. Along such a line we write $\phi(\vec{x}) = u(r)/r$ with $u(0) = 0$. We consider first the special case when when U is a delta-function at some radius $R \geq R_0$, i.e.,

$$U(r) = \frac{1}{R^2}\delta(r - R). \tag{3.5}$$

For such U the analog of (3.4) along the radial line is

$$\int_0^{R_1} \{\mu[u'(r) - (u(r)/r)]^2 + \tfrac{1}{2}v(r)|u(r)|^2\}dr \geq \begin{cases} 0 & \text{if } R_1 < R \\ \mu a|u(R)|^2/R^2 & \text{if } R \leq R_1 \end{cases} \tag{3.6}$$

where R_1 is the length of the radial line segment in $\mathcal{B}$. The case $R_1 < R$ is trivial, because $\mu|\partial\psi/\partial r|^2 + \frac{1}{2}v|\psi|^2 \geq 0$. (Note that positivity of v is used here.) If $R \leq R_1$ we consider the integral on the the left side of (3.6) from 0 to R instead of R_1 and minimize it under the boundary condition that $u(0) = 0$ and $u(R)$ is a fixed constant. Since everything is homogeneous in u we may normalize this value to $u(R) = R - a$. This minimization problem leads to the zero energy scattering equation (1.4). Since v is positive, the solution is a true minimum and not just a stationary point.

Because $v(r) = 0$ for $r > R_0$ the solution, u_0, satisfies $u_0(r) = r - a$ for $r > R_0$. By partial integration,

$$\int_0^{R} \{\mu[u_0'(r) - (u_0(r)/r)]^2 + \tfrac{1}{2}v(r)|u_0(r)|^2\}dr = \mu a|R - a|^2/R^2. \tag{3.7}$$

But $|R - a|^2/R^2$ is precisely the right side of (3.6) if u satisfies the normalization condition.

This derivation of (3.4) for the special case (3.5) implies the general case, because every U can be written as a superposition of δ-functions, $U(r) = \int R^{-2}\delta(r-R)\,U(R)R^2dR$, and $\int U(R)R^2dR \leq 1$ by assumption. $\square$

By dividing Λ for given points $\vec{x}_1,\ldots,\vec{x}_N$ into Voronoi cells $\mathcal{B}_i$ that contain all points closer to $\vec{x}_i$ than to $\vec{x}_j$ with $j \neq i$ (these cells are star shaped w.r.t. $\vec{x}_i$, indeed convex), the following corollary of Lemma 3.3 can be derived in the same way as the corresponding Eq. (28) in [10].

Corollary 3.4 *For any U as in Lemma 3.3*

$$H_N \geq \mu a W \tag{3.8}$$

with

$$W(\vec{x}_1,\ldots,\vec{x}_N) = \tfrac{1}{2}\sum_{i=1}^{N} U(t_i), \tag{3.9}$$

where t_i is the distance of $\vec{x}_i$ to its nearest neighbor among the other points $\vec{x}_j$, $j=1,\ldots,N$, i.e.,

$$t_i(\vec{x}_1,\ldots,\vec{x}_N) = \min_{j,\, j\neq i} |\vec{x}_i - \vec{x}_j|. \tag{3.10}$$

(Note that t_i has here a slightly different meaning than in (2.5), where it denoted the distance to the nearest neighbor among the $\vec{x}_j$ with $j \leq i-1$.)

Dyson considers in [10] a one parameter family of U's that is essentially the same as the following choice, which is convenient for the present purpose:

$$U_R(r) = \begin{cases} \frac{1}{3}(R^3 - R_0^3)^{-1} & \text{for } R_0 < r < R \\ 0 & \text{otherwise.} \end{cases} \tag{3.11}$$

We denote the corresponding interaction (3.9) by W_R. For the hard core gas one obtains

$$E(N,L) \geq \sup_R \inf_{(\vec{x}_1,\ldots,\vec{x}_N)} \mu a W_R(\vec{x}_1,\ldots,\vec{x}_N) \tag{3.12}$$

where the infimum is over $(\vec{x}_1,\ldots,x_N) \in \Lambda^N$ with $|\vec{x}_i - \vec{x}_j| \geq R_0 = a$, because of the hard core. At fixed R simple geometry gives

$$\inf_{(\vec{x}_1,\ldots,\vec{x}_N)} W_R(\vec{x}_1,\ldots,\vec{x}_N) \geq \left(\frac{A}{R^3} - \frac{B}{\rho R^6}\right) \tag{3.13}$$

with certain constants A and B. An evaluation of these constants gives Dyson's bound

$$E(N,L)/N \geq \frac{1}{10\sqrt{2}} 4\pi\mu\rho a. \tag{3.14}$$

The main reason this method does not give a better bound is that R must be chosen quite big, namely of the order of the mean particle distance $\rho^{-1/3}$, in order to guarantee that the spheres of radius R around the N points overlap. Otherwise the infimum of W_R will be zero. But large R means that W_R is small. It should also be noted that this method does not work for potentials other than hard spheres: If $|\vec{x}_i - \vec{x}_j|$ is allowed to be less than R_0, then the right side of (3.12) is zero because $U(r) = 0$ for $r < R_0$.

For these reasons we take another route. We still use Lemma 3.4 to get into the soft potential regime, but we do *not* sacrifice *all* the kinetic energy as in (3.8). Instead we write, for $\varepsilon > 0$

$$H_N = \varepsilon H_N + (1-\varepsilon) H_N \geq \varepsilon T_N + (1-\varepsilon) H_N \tag{3.15}$$

with $T_N = -\sum_i \Delta_i$ and use (3.8) only for the part $(1-\varepsilon)H_N$. This gives

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\mu a W_R. \tag{3.16}$$

We consider the operator on the right side from the viewpoint of first order perturbation theory, with εT_N as the unperturbed part, denoted H_0.

The ground state of H_0 in a box of side length L is $\Psi_0(\vec{x}_1, \ldots, \vec{x}_N) \equiv L^{-3N/2}$ and we denote expectation values in this state by $\langle\cdot\rangle_0$. A computation, cf. Eq. (21) in [3], gives

$$\begin{aligned} 4\pi\rho\left(1-\tfrac{1}{N}\right) &\geq \langle W_R\rangle_0/N \qquad\qquad (3.17)\\ &\geq 4\pi\rho\left(1-\tfrac{1}{N}\right)\left(1-\tfrac{2R}{L}\right)^3\left(1+4\pi\rho(1-\tfrac{1}{N})(R^3-R_0^3)/3)\right)^{-1}. \end{aligned}$$

The rationale behind the various factors is as follows: $(1-\frac{1}{N})$ comes from the fact that the number of pairs is $N(N-1)/2$ and not $N^2/2$, $(1-2R/L)^3$ takes into account the fact that the particles do not interact beyond the boundary of Λ, and the last factor measures the probability to find another particle within the interaction range of the potential U_R for a given particle.

The first order result (3.17) looks at first sight quite promising, for if we let $L \to \infty$, $N \to \infty$ with $\rho = N/L^3$ fixed, and subsequently take $R \to \infty$, then $\langle W_R\rangle_0/N$ converges to $4\pi\rho$, which is just what is desired. But the first order result (3.17) is not a rigorous bound on $E_0(N,L)$, we need *error estimates*, and these will depend on ε, R and L.

We now recall *Temple's inequality* [13] for the expectations values of an operator $H = H_0+V$ in the ground state $\langle\cdot\rangle_0$ of H_0. It is a simple consequence of the operator inequality

$$(H - E_0)(H - E_1) \geq 0 \tag{3.18}$$

for the two lowest eigenvalues, $E_0 < E_1$, of H and reads

$$E_0 \geq \langle H\rangle_0 - \frac{\langle H^2\rangle_0 - \langle H\rangle_0^2}{E_1 - \langle H\rangle_0} \tag{3.19}$$

provided $E_1 - \langle H\rangle_0 > 0$. Furthermore, if $V \geq 0$ we may use $E_1 \geq E_1^{(0)}=$ second lowest eigenvalue of H_0 and replace E_1 in (3.19) by $E_1^{(0)}$.

From (3.19) we get the estimate

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1 - \mathcal{E}(\rho, L, R, \varepsilon)) \tag{3.20}$$

with

$$1 - \mathcal{E}(\rho, L, R, \varepsilon) = (1-\varepsilon)\left(1 - \frac{1}{\rho L^3}\right)\left(1 - \frac{\mu a\big(\langle W_R^2\rangle_0 - \langle W_R\rangle_0^2\big)}{\langle W_R\rangle_0\big(E_1^{(0)} - \mu a\langle W_R\rangle_0\big)}\right). \tag{3.21}$$

To evaluate this further one may use the estimates (3.17) and the bound

$$\langle W_R^2\rangle_0 \leq 3\frac{N}{R^3 - R_0^3}\langle W_R\rangle_0 \tag{3.22}$$

which follows from $U_R^2 = 3^{-1}(R^3 - R_0^3)^{-1}U_R$ together with the Cauchy-Schwarz inequality. A glance at the form of the error term reveals, however, that it is *not* possible here to take the thermodynamic limit $L \to \infty$ with ρ fixed: We have $E_1^{(0)} = \varepsilon\pi\mu/L^2$ (this is the kinetic energy of a *single* particle in the first excited state in the box), and the factor $E_1^{(0)} - \mu a\langle W_R\rangle_0$ in the denominator in (3.21) is, up to unimportant constants and lower order terms, $\sim (\varepsilon L^{-2} - a\rho^2 L^3)$. Hence the denominator eventually becomes negative and Temple's inequality looses its validity if L is large enough.

As a way out of this dilemma we divide the big box Λ into cubic *cells* of side length ℓ that is kept *fixed* as $L \to \infty$. The number of cells, L^3/ℓ^3, on the other hand, increases with L. The N particles are distributed among these cells, and we use (3.21), with L replaced by ℓ, N by the particle number, n, in a cell and ρ by n/ℓ^3, to estimate the energy in each cell with *Neumann* conditions on the boundary. This boundary condition leads to lower energy than any other boundary condition. For each distribution of the particles we add the contributions from the cells, neglecting interactions across boundaries. Since $v \geq 0$ by assumption, this can only lower the energy. Finally, we minimize over all possible choices of the particle numbers for the various cells adding up to N. The energy obtained in this way is a lower bound to $E_0(N, L)$, because we are effectively allowing discontinuous test functions for the quadratic form given by H_N.

In mathematical terms, the cell method leads to

$$E_0(N,L)/N \geq (\rho\ell^3)^{-1} \inf \sum_{n \geq 0} c_n E_0(n,\ell) \tag{3.23}$$

where the infimum is over all choices of coefficients $c_n \geq 0$ (relative number of cells containing exactly n particles), satisfying the constraints

$$\sum_{n\geq 0} c_n = 1, \qquad \sum_{n \geq 0} c_n n = \rho\ell^3. \tag{3.24}$$

The minimization problem for the distributions of the particles among the cells would be easy if we knew that the ground state energy $E_0(n, \ell)$ (or a good lower bound to it) were convex in n. Then we could immediately conclude that it is best to have the particles as evenly distributed among the boxes as possible, i.e., c_n would be zero except for the n equal to the integer closest to $\rho\ell^3$. This would give

$$\frac{E_0(N,L)}{N} \geq 4\pi\mu a\rho\,(1 - \mathcal{E}(\rho, \ell, R, \varepsilon)) \tag{3.25}$$

i.e., replacement of L in (3.20) by ℓ, which is independent of L. The blow up of $\mathcal{E}$ for $L \to \infty$ would thus be avoided.

Since convexity of $E_0(n,\ell)$ is not known (except in the thermodynamic limit) we must resort to other means to show that $n = O(\rho\ell^3)$ in all boxes. The rescue comes from *superadditivity* of $E_0(n,\ell)$, i.e., the property

$$E_0(n + n', \ell) \geq E_0(n,\ell) + E_0(n',\ell) \tag{3.26}$$

which follows immediately from $v \geq 0$ by dropping the interactions between the n particles and the n' particles. The bound (3.26) implies in particular that for any $n, p \in \mathbb{N}$ with $n \geq p$

$$E(n, \ell) \geq [n/p]\, E(p, \ell) \geq \frac{n}{2p} E(p, \ell) \tag{3.27}$$

since the largest integer $[n/p]$ smaller than n/p is in any case $\geq n/(2p)$.

The way (3.27) is used is as follows: Replacing L by ℓ, N by n and ρ by n/ℓ^3 in (3.20) we have for fixed R and ε

$$E_0(n, \ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1) K(n, \ell) \tag{3.28}$$

with a certain function $K(n, \ell)$ determined by (3.21). We shall see that K is monotonously decreasing in n, so that if $p \in \mathbb{N}$ and $n \leq p$ then

$$E_0(n, \ell) \geq \frac{4\pi\mu a}{\ell^3} n(n-1) K(p, \ell). \tag{3.29}$$

We now split the sum in (3.23) into two parts. For $n < p$ we use (3.29), and for $n \geq p$ we use (3.27) together with (3.29) for $n = p$. The task is thus to minimize

$$\sum_{n<p} c_n n(n-1) + \tfrac{1}{2} \sum_{n \geq p} c_n n(p-1) \tag{3.30}$$

subject to the constraints (3.24). Putting

$$k := \rho\ell^3 \quad \text{and} \quad t := \sum_{n<p} c_n n \leq k \tag{3.31}$$

we have $\sum_{n \geq p} c_n n = k - t$, and since $n(n-1)$ is convex in n, and $\sum_{n<p} c_n \leq 1$ the expression (3.30) is

$$\geq t(t-1) + \tfrac{1}{2}(k-t)(p-1). \tag{3.32}$$

We have to minimize this for $1 \leq t \leq k$. If $p \geq 4k$ the minimum is taken at $t = k$ and is equal to $k(k-1)$. Altogether we have thus shown that

$$\frac{E_0(N, L)}{N} \geq 4\pi\mu a\rho \left(1 - \frac{1}{4\rho\ell^3}\right) K(4\rho\ell^3, \ell). \tag{3.33}$$

What remains is to take a closer look at $K(4\rho\ell^3,\ell)$, which depends on the parameters ε and R besides ℓ, and choose the parameters in an optimal way. From (3.21), using (3.17) and (3.22) we obtain

$$K(n,\ell) = (1-\varepsilon)\left(1 - \frac{3}{\pi}\frac{an}{(R^3-R_0^3)(\varepsilon\ell^{-2}-4a\ell^{-3}n(n-1))}\right). \tag{3.34}$$

The estimate (3.28) with this K is valid as long as the denominator in (3.34) is ≥ 0, and in order to have a formula for all n we can take 0 as a trivial lower bound in other cases or when (3.28) is negative. As required for (3.29), K is monotonously decreasing in n. We now insert $n = 4\rho\ell^3$ and obtain

$$K(4\rho\ell^3,\ell) \geq (1-\varepsilon)\left(1 - \frac{\ell^3}{(R^3-R_0^3)}\frac{(\text{const.})Y}{(\varepsilon(a/\ell)^2-(\text{const.})Y^2(\ell/a)^3)}\right) \tag{3.35}$$

with $Y = 4\pi\rho a^3/3$ as before. Also, the factor

$$\left(1-\frac{1}{4\rho\ell^3}\right) = (1-(\text{const.})Y^{-1}(a/\ell)^3) \tag{3.36}$$

in (3.33) (which is the ratio between $n(n-1)$ and n^2) must not be be forgotten. We now make the ansatz

$$\varepsilon \sim Y^\alpha, \quad a/\ell \sim Y^\beta, \quad (R^3-R_0^3)/\ell^3 \sim Y^\gamma \tag{3.37}$$

with exponents α, β and γ that we choose in an optimal way. The conditions to be met are as follows:

- $\varepsilon(a/\ell)^2 - (\text{const.})Y^2(\ell/a)^3 > 0$. This holds for all small enough Y, provided $\alpha + 5\beta < 2$.
- $\alpha > 0$ in order that $\varepsilon \to 0$ for $Y \to 0$.
- $3\beta - 1 > 0$ in order that $Y^{-1}(a/\ell)^3 \to 0$ for for $Y \to 0$.
- $1 - \alpha - 2\beta - \gamma > 0$ to control the second factor in (3.35).

Taking

$$\alpha = 1/17, \quad \beta = 6/17, \quad \gamma = 3/17 \tag{3.38}$$

all these conditions are satisfied, and

$$\alpha = 3\beta - 1 = 1 - \alpha - 2\beta - \gamma = 1/17. \tag{3.39}$$

This completes the proof of Theorems 3.1 and 3.2, for the case of potentials with finite range. By optimizing the proportionality constants in (3.37) one can show that $C = 8.9$ is possible in Theorem 1.1 [5]. The extension to potentials of infinite range decreasing faster than $1/r^3$ at infinity is obtained by approximation by finite range potentials, controlling the change of the scattering length as the cut-off is removed. See Appendix B in [4] for details. A slower decrease than $1/r^3$ implies infinite scattering length.

□

The exponents (3.38) mean in particular that

$$a \ll R \ll \rho^{-1/3} \ll \ell \ll (\rho a)^{-1/2}, \tag{3.40}$$

whereas Dyson's method required $R \sim \rho^{-1/3}$ as already explained. The condition $\rho^{-1/3} \ll \ell$ is required in order to have many particles in each box and thus $n(n-1) \approx n^2$. The condition $\ell \ll (\rho a)^{-1/2}$ is necessary for a spectral gap gap $\gg e_0(\rho)$ in Temple's inequality. It is also clear that this choice of ℓ would lead to a far too big energy and no bound for $e_0(\rho)$ if we had chosen Dirichlet instead of Neumann boundary conditions for the cells. But with the latter the method works!

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