# The leading order lower bound for the ground state energy of a 3D dilute Bose gas

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In this little review we will derive a leading order lower bound for the ground state energy of a dilute Bose Gas in the Thermodynamic limit. The argument presented here is a re-elaboration of [LY98] and of Section 2.2 of [Lie+05].

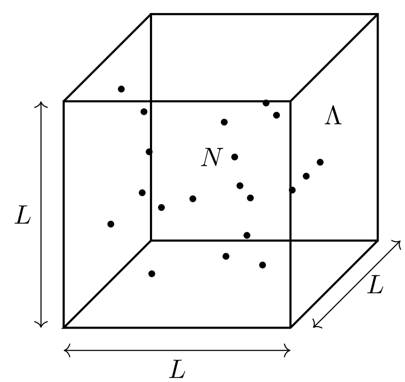


Figure 1: The "thermodynamic" box $\Lambda$.

More precisely we are lower bounding the ground state energy of the following Hamiltonian:

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

acting on $L^2(\Lambda)^{\otimes_s N}$, where $\Lambda$ is a Neumann box with sidelength $L$. The potential appearing in (1) is assumed to be *radial*, *positive* and *compactly supported*.

The diluteness condition can be modeled by the following relation between the mean interparticle distance $\rho^{-1/3}$ (where $\rho := N/L^3$ indicates the particle density) and the *scattering lenght* $\mathfrak{a}$:

$$\rho^{-1/3} \gg \mathfrak{a}\,,$$

meaning that the gas is so sparse that interaction within particles is very sporadic. Such a relation between $\rho^{-1/3}$ and $\mathfrak{a}$ can again be turned into a smallness condition for the dimensionless quantity $\rho\,\mathfrak{a}^3 \ll 1$, the so-called *diluteness parameter*.

Our goal result is summarized by the following theorem:

**Theorem 1** (Lower Bound for the Ground State Energy of a 3D Dilute Bose gas)**.** *For a positive potential with compact support $v$, where we denote with $R_0$ its radius of support, one has that the ground state energy of* (1) *with Neumann boundary conditions on the box satisfies:*

$$\frac{E_{GS}(N,L)}{N} \geq 4\pi\rho\,\mathfrak{a}(1 - C(\rho\,\mathfrak{a}^3)^{1/17})\,. \tag{2}$$

## 1 Preliminary Lemmas

**Lemma 2** (Dyson's Lemma [Dys57])**.** *Let $v$ be a radial, positive potential with compact support. Let $R_0$ be the radius of support of such a potential. Let $U$ be any positive radial function satisfying the following conditions*

- $\int_{\mathbb{R}^+} U(r) r^2\,\mathrm{d}r \leq 1$*;*
- $U(r) \equiv 0$ *for* $r \leq R_0$ *.*

*Considering a set $\mathcal{B} \subset \mathbb{R}^3$ starshaped with respect to zero, then one has for all differentiable functions $\psi$:*

$$\int_{\mathcal{B}} \mathrm{d}x \left(|\nabla\psi|^2 + \frac{1}{2}v|\psi|^2\right) \geq \mathfrak{a}\int_{\mathcal{B}} \mathrm{d}x\,U|\psi|^2\,. \tag{3}$$

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*Proof.* In order to prove the lemma, it is sufficient to prove it for the particular case

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

for $R \geq R_0$. In fact any other $U$ that satisfies the hypothesis above can be reconstructed as a *superposition* of $\delta$-functions:

$$\int_{\mathbb{R}^+} \mathrm{d}R\, \frac{1}{R^2}\delta(r-R)U(R)R^2 = U(r)\,.$$

So proving the above inequality (3) for the particular case would yield for the general case:

$$\int_{\mathcal{B}} \mathrm{d}x\, \left(|\nabla\psi|^2 + \frac{1}{2}v|\psi|^2\right) \geq \mathfrak{a}\int_{\mathcal{B}} \mathrm{d}x\, \frac{1}{R^2}\delta(r-R)|\psi|^2 \geq \mathfrak{a}\int_{\mathbb{R}^+} \mathrm{d}R\, R^2 U(R)\int_{\mathcal{B}} \mathrm{d}x\, \frac{1}{R^2}\delta(r-R)|\psi|^2\,,$$

since $\int_{\mathbb{R}^+} U(r)r^2\,\mathrm{d}r \leq 1$.

So, given this remark we focus on the particular case of the $\delta$ function.

Expanding the gradient in spherical coordinates one can easily obtain the bound $|\nabla\psi| \geq \left|\frac{\partial\psi}{\partial r}\right|$ and hence get

$$\int_{\mathcal{B}} \mathrm{d}x\, \left(|\nabla\psi|^2 + \frac{1}{2}v|\psi|^2\right) \geq \int_{\mathcal{B}} \mathrm{d}x\, \left(\left|\frac{\partial\psi}{\partial r}\right|^2 + \frac{1}{2}v|\psi|^2\right)\,,$$

so in order to prove the lemma we can substitute this smaller integral involving the radial part of the gradient on the LHS of (3). This substitution makes the problem completely radial (remember the assumptions on the potential). So in order to prove the claimed inequality it suffices to prove it on a radial line connecting 0 to the border of $\mathcal{B}$ at fixed angular variable, for every choice of angular variables.

To make the calculations cleaner we define implicitly the function $u$ as $\psi(x) = \frac{u(r)}{r}$ with $u(0) = 0$. So in this setting the inequality that we want to prove becomes:

$$\int_0^{R_1} \mathrm{d}r\, \left[\left(u'(r) - \frac{u(r)}{r}\right)^2 + \frac{1}{2}v(r)|u(r)|^2\right] \geq \begin{cases} 0 & \text{if } R_1 < R \\ \mathfrak{a}\,\frac{|u(R)|^2}{R^2} & \text{if } R \leq R_1 \end{cases}\,, \tag{4}$$

where $R_1$ is the length of the line connecting 0 to the border of $\mathcal{B}$ at the fixed angular variables that we are considering.

The case $R_1 < R$ is trivial since the integrand is positive. For the other case using again the fact that the integrand is positive one has that $\int_0^{R_1}(\dots) \geq \int_0^R(\dots)$, so we will restrict our integral up until the value $R$.

Hence in order to get a good lower bound we minimize the integral that appears on the LHS of (4) with $R_1 = R$ and the boundary conditions $u(0) = 0$, $u(R) = C$. Since the problem is homogeneous in $u$ we are able to choose whatever $C$ we please. For reasons that will become apparent soon, we will choose $C = R - \mathfrak{a}$.

By doing the first variation of the integral that appears on the LHS of (4) one obtains the *radial version* of the zero energy scattering equation, and with our choice of normalization for $u(R)$ we get exactly the asymptotic behaviour $u^{(\infty)}(r) = r - \mathfrak{a}$. Integrating by parts a couple of times in a clever way one gets:

$$\int_0^{R} \mathrm{d}r\, \left[\left(u'(r) - \frac{u(r)}{r}\right)^2 + \frac{1}{2}v(r)|u(r)|^2\right] = \mathfrak{a}\,\frac{|R-\mathfrak{a}\,|}{R} \geq \mathfrak{a}\,\frac{(R-\mathfrak{a})^2}{R^2}\,.$$

But the RHS of the previous equation is exactly what we wanted (i.e. what one gets integrating the special case of U that we have chosen). This concludes the proof of the Lemma.

QED

A corollary of Dyson's Lemma will prove to be extremely useful in the analysis that follows.

**Corollary 2.1.** *For any $U$ that satisfies the hypothesis of Lemma 2, defining the multiplication operator*

$$W(x_1, x_2, \dots, x_N) = \sum_{i=1}^{N} U(t_i)\,, \tag{5}$$

*where $t_i$ is the distance of $x_i$ from its nearest neighbor among the other $x_j$, i.e. to be more explicit:*

$$t_i(x_1, \dots, x_N) = \min_{\substack{j \in \{1,\dots,N\} \\ j \neq i}} |x_i - x_j| \,,$$

*one gets the operator bound*

$$H_N \geq \mathfrak{a} W \,. \tag{6}$$

*Proof.* We recall that:

$$\langle \Psi \,,\, H_N \Psi \rangle = \int_{\mathbb{R}^{3N}} \mathrm{d}x_1 \dots \mathrm{d}x_N \left( \sum_{i=1}^{N} |\nabla_{x_i} \Psi|^2 + \sum_{i<j} v_{ij} |\Psi|^2 \right) .$$

Now we temporarily fix the variables $x_2, \dots, x_N$ and regard $\Psi$ as $\Psi(x_1)$ i.e. as a function of only the first variable.

Then we divide the box $|\Lambda|$ in the Voronoi Cells generated by the configuration of the fixed particles $x_2, \dots, x_N$. We call the Voronoi cell related to particle $j$ $\mathcal{B}_j$. By construction $\mathcal{B}_j$ is star-shaped with respect to $x_j$. So, considering $r = |x_1 - x_j|$ only when $x_1$ is in $\mathcal{B}_j$ (i.e. $r = t_1$) one gets, using Lemma 2:

$$\int_{\mathcal{B}_j} \mathrm{d}x_1 \left( |\nabla_{x_1} \Psi|^2 + \frac{1}{2} v_{1j} |\Psi|^2 \right) \geq \mathfrak{a} \int_{\mathcal{B}_j} \mathrm{d}x_1 \, U(t_1) |\Psi|^2 \,.$$

We put the $1/2$ in front of the potential contribution, because the choice of $x_1$ is not essential and one can do this inequality with every $x_j$. So we split $v_{ij}$ in half. One half is used when we derive with $x_i$ and we consider the Voronoi cell $\mathcal{B}_j$ and the other half is considered when the role of the two indices is inverted.

Indicating with $\mathrm{nn}(i)$ the index of the nearest neighbor particle to $i$, one can sum over all $j \neq 1$ the inequalities we found before to get:

$$\int_{\mathbb{R}^3} \mathrm{d}x_1 \left( |\nabla_{x_1} \Psi|^2 + \frac{1}{2} v_{1,\mathrm{nn}(1)} |\Psi|^2 \right) \geq \mathfrak{a} \int_{\mathbb{R}^3} \mathrm{d}x_1 \, U(t_1) |\Psi|^2 \,,$$

and since $\sum_{j \neq 1} v_{1j} \geq v_{1,\mathrm{nn}(1)}$ one finds:

$$\int_{\mathbb{R}^3} \mathrm{d}x_1 \left( |\nabla_{x_1} \Psi|^2 + \frac{1}{2} \sum_{k \neq 1} v_{1k} |\Psi|^2 \right) \geq \mathfrak{a} \int_{\mathcal{B}_j} \mathrm{d}x_1 \, U(t_1) |\Psi|^2 \,.$$

As we remarked before, the choice of $x_1$ was not special at all, so a similar inequality holds up for all $x_i$. Hence, integrating those inequalities also with respect to the other variables and summing over all $i$ one gets:

$$\langle \Psi \,,\, H_N \Psi \rangle \geq \mathfrak{a} \langle \Psi \,,\, W \Psi \rangle \,,$$

where $W$ is the one defined in the hypothesis of the theorem. The inequality above means exactly $H_N \geq \mathfrak{a} W$, since it holds for an arbitrary $\Psi$ for which the action of the two operators is well defined, thus proving the corollary. QED

*Remark* 1.1. The corollary tells us that the Hamiltonian $H_N$ is always bounded from below by a suitable nearest neighbor potential.

The last main ingredient for the lower bound proof is the so-called *Temple's Inequality*, an inequality that is extremely useful for "perturbation theory" kind of problems.

Consider a Hamiltonian $H$ of the type $H = H_0 + V$. Usually one physically thinks of $H_0$ as the *unperturbed* Hamiltonian and of $V$ as an added perturbation. In perturbation theory, usually one tries to study the spectrum of $H$ by perturbing the spectrum of $H_0$. Let $\psi_0$ be the ground state of $H_0$, and let $\langle \cdot \rangle_0$ denote the expectation value of $\cdot$ with respect to $\psi_0$.

One has the trivial operator inequality:

$$(H - E_0)(H - E_1) \geq 0 \,,$$

where $E_0$ and $E_1$ are, respectively, the lowest and the second lowest eigenvalue of $H$. Then, taking the expectation value with respect to $\psi_0$ of the previous operator inequality, under the condition that $E_1 - \langle H \rangle_0 > 0$, one gets the following:

$$E_0 \geq \langle H \rangle_0 - \frac{\langle H^2 \rangle_0 - \langle H \rangle_0^2}{E_1 - \langle H \rangle_0} \,. \tag{7}$$

One notices that whenever $V$ is positive then the second lowest eigenvalue of $H_0$ is smaller than the second lowest eigenvalue of $H$, i.e. $E_1 \geq E_1^{(0)}$. From this one gets *Temple's inequality*:

$$E_0 \geq \langle H \rangle_0 - \frac{\langle H^2 \rangle_0 - \langle H \rangle_0^2}{E_1^{(0)} - \langle H \rangle_0}, \tag{8}$$

valid under the condition $E_1^{(0)} - \langle H \rangle_0 > 0$.

# 2 (The worse version of) Dyson Lower Bound

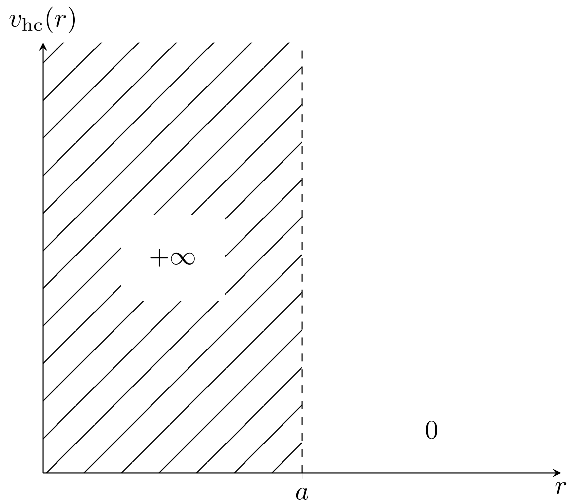


Figure 2: A graphical representation of the *hard core* potential

To get a feeling on how those preliminary lemmas can be used in the computation of a leading order lower bound for the ground state energy per particle in the thermodynamic limit, we will give a simplified version of Dyson's proof of its lower bound. We will get the main order term with the wrong constant in front. This will be a starting point for the construction of a proper lower bound proof.

Dyson studied a particular case, the so called *hard-core potential* $v_{\mathrm{hc}}$ represented in Figure 2, and in the same paper where he proved the upper bound [Dys57] he managed to prove this weaker lower bound. We notice that in the case of the hardcore potential, $R_0 = \mathfrak{a}$. We will also only consider that potential for this section.

Dyson chose a one parameter family of functions that satisfy the hypothesis of Lemma 2 $\{U_R\}_{R\in(R_0,\infty)}$ that is very similar to the following one (chosen in [LY98; Lie+05]):

$$U_R(r) := \begin{cases} \dfrac{3}{R^3 - R_0^3} & \text{for } R_0 < r < R \\ \\ 0 & \text{otherwise} \end{cases} . \tag{9}$$

By indicating as $W_R$ the nearest neighbor potential of Corollary 2.1 related to $U_R$ and using the result of that corollary to bound the full hamiltonian, one gets the following inequality:

$$\begin{aligned} E_{GS}(N, L) &\geq \sup_R \inf \operatorname{spec}(\mathfrak{a}\, W_R) = \\ &= \mathfrak{a} \sup_R \inf_{\substack{(x_1,\ldots,x_N)\in\Lambda^N \\ |x_i - x_j| \geq \mathfrak{a}}} W_R(x_1, \ldots, x_n)\,. \end{aligned}$$

So, we need to study the infimum of $W_R$ over all possible configurations given $R$ fixed.

Given (9) we see how obtaining the infimum of the spectrum of that operator is related to placing balls in a box. One starts by placing as many balls with radius $R/2$ in the box $\Lambda$ without overlap. But if the balls that one has to place are too many then adding the remaining balls (still, compatibly with the hardcore condition) forces some overlaps. The infimum configuration is obtained by placing the particles positions at the centers of those balls. Defining as $N_0$ the number of balls you can put in without any overlap and as $N$ the total number of particles one gets that:

$$\begin{aligned} \inf_{\substack{(x_1,\ldots,x_N)\in\Lambda^N \\ |x_i - x_j| \geq \mathfrak{a}}} W_R(x_1, \ldots, x_n) =& (N - N_0)\frac{3}{R^3 - R_0^3} \geq \left(\rho L^3 - \frac{L^3}{\frac{4\pi}{3}\left(\frac{R}{2}\right)^3}\right)\frac{3}{R^3 - R_0^3} \geq \\ \geq& 3\rho L^3 \left(1 - \frac{6}{\pi \rho R^3}\right)\frac{1}{R^3}\,, \end{aligned}$$

where we used the fact that $N_0 \leq \dfrac{L^3}{\frac{4\pi}{3}\left(\frac{R}{2}\right)^3}$.

Maximizing the resulting RHS with respect to $R$ one gets that $R_{\max} = \left(\dfrac{12}{\pi\rho}\right)^{1/3}$. And thus by plugging in the expression of $R_{\max}$ in, one gets:

$$E_{GS}(L,N) \geq \frac{1}{32} 4\pi\rho\,\mathfrak{a}\,N\,. \tag{10}$$

Dyson used a slightly different $U_R$ and some finer upper bound for $N_0$ using the theory of the sphere packing problem, so he got a better result:

$$E_{GS}(L,N) \geq \frac{1}{10\sqrt{2}} 4\pi\rho\,\mathfrak{a}\,N\,, \tag{11}$$

however, since we are later giving a better lower bound, we didn't bother including the optimal estimates, but we focused on giving out the main idea of his proof.

This Dyson bound will be our starting point. We would like a better way to refine it. The computation showed us that using Corollary 2.1 right off the bat is too crude of an approximation.

# 3 Towards the right idea

In the last section we saw that using Corollary 2.1 to bound the Hamiltonian in its entirety makes us lose too much, so maybe one can use that result only to lower bound *part* of it.

Obviously then, for every $0 < \varepsilon < 1$: $H_N = \varepsilon H_N + (1-\varepsilon)H_N \geq \varepsilon T_N + (1-\varepsilon)H_N$, where $T_N$ denotes the kinetic energy. So using the bound only on the term multiplied by $(1-\varepsilon)$:

$$H_N \geq \varepsilon T_N + (1-\varepsilon)\,\mathfrak{a}\,W_R =: \tilde{H}_N\,,$$

where we used the same $U_R$ as before for the definition of $W_R$.

Together with this bound on the operator $H_N$, we would also like to use *Temple's inequality* (8). So it will become handy to calculate or to appropriately bound the factor $\langle W_R\rangle_{\Psi_0}$, where $\Psi_0$ is the ground state of $\varepsilon T_N$ (our $H_0$), i.e. $\Psi_0(x_1,\ldots,x_N) = L^{-3N/2}$. For the sake of brevity we will write $X$ to indicate the set $\{x_1,\ldots,x_N\}$ and $X^{(i)}$ to indicate $\{x_1,\ldots,x_{i-1},x_{i+1},\ldots,x_N\}$. So:

$$\frac{\langle W_R\rangle_{\Psi_0}}{N} = \frac{1}{NL^{3N}}\sum_{i=1}^{N}\int_{\Lambda}\mathrm{d}x_i\int_{\Lambda^{N-1}}\mathrm{d}X^{(i)}\,U(t_i)\,,$$

to compute the integrals above one can estimate the probability that at least one particle among the $N-1$ remaining is in the annulus $R_0 < |x_i - x| < R$, then multiply this probability by the non zero value of $U_R$, i.e. $3/(R^3 - R_0^3)$ and by the mass carried by the integrals.

Unfortunately, computing this probability is challenging due to the presence of the Neumann boundary conditions on the box. So, in order to make such a computation easier, instead of going for an exact result we opt for a good lower and upper bound. In both cases we would like to make the probability estimate that we need easy, by removing the strange terms due to the boundary condition.

The trick is the following:

- For an upper bound, since the integrand is positive, one can extend the integral in $\mathrm{d}x_i$ to a slightly bigger box $\Lambda_B$ with the same center as $\Lambda$ but with sides of length $(L+2R)$;
- For a lower bound one does the same but with a smaller box $\Lambda_S$ with sidelength $(L-2R)$.

This trick allows the computation of the wanted probability to be much easier. Let's look at the upper bound case for reference. The probability that particle $i$ is in the aforementioned annulus relative to particle $j$ is:

$$P_u = \frac{\frac{4\pi}{3}(R^3 - R_0^3)}{(L+2R)^3}\,,$$

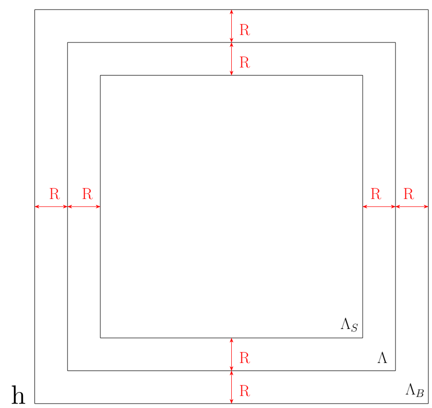


Figure 3: The modified boxes for computing probabilities

while, the same probability for the lower bound is

$$P_\ell = \frac{\frac{4\pi}{3}(R^3 - R_0^3)}{L^3}\,.$$

Given these two results, the probability that at least one particle is in the Goldilocks zone is

$$Q_{u/\ell} = 1 - (1 - P_{u/\ell})^{N-1}\,.$$

From this result one gets:

$$\frac{(L-2R)^3}{L^3} Q_\ell \frac{3}{R^3 - R_0^3} \leq \frac{\langle W_R \rangle_{\Psi_0}}{N} \leq \frac{(L+2R)^3}{L^3} Q_u \frac{3}{R^3 - R_0^3}\,,$$

and thus, using the inequalities $(1 - \alpha x) \leq (1-x)^\alpha \leq (1 + \alpha x)^{-1}$, where the lower bound holds for $\alpha \geq 1$, that are in general only valid for x sufficiently small, then:

$$4\pi\rho \left(1 - \frac{1}{N}\right)\left(1 - \frac{2R}{L}\right)^3 \left(1 + \frac{4\pi\rho}{3}(R^3 - R_0^3)\right)^{-1} \leq \frac{\langle W_R \rangle_{\Psi_0}}{N} \leq 4\pi\rho\left(1 - \frac{1}{N}\right)\,. \tag{12}$$

This upper and lower bound that we just derived are really good since they tell us that in the thermodynamic limit $\frac{\langle W_R \rangle_{\Psi_0}}{N}$ goes to $4\pi\rho$.

Hence, applying Temple's inequality:

$$\frac{E_{GS}(N,L)}{N} \geq \frac{E_{GS}^{(\tilde{H}_N)}(N,L)}{N} \geq \frac{\langle \tilde{H}_N \rangle_{\Psi_0}}{N} \left(1 - \frac{\langle \tilde{H}_N^2 \rangle_{\Psi_0} - \langle \tilde{H}_N \rangle_{\Psi_0}^2}{\langle \tilde{H}_N \rangle_{\Psi_0}\left(E_1^{(0)} - \langle \tilde{H}_N \rangle_{\Psi_0}\right)}\right) \geq$$

$$\geq (1-\varepsilon)\,\mathfrak{a}\,\frac{\langle W_R \rangle_{\Psi_0}}{N}\left(1 - \frac{\mathfrak{a}\left(\langle W_R^2 \rangle_{\Psi_0} - \langle W_R \rangle_{\Psi_0}^2\right)}{\langle W_R \rangle_{\Psi_0}\left(E_1^{(0)} - \mathfrak{a}\langle W_R \rangle_{\Psi_0}\right)}\right)\,,$$

and thus, using (12), one gets:

$$\frac{E_{GS}(N,L)}{N} \geq 4\pi\rho\,\mathfrak{a}\,(1 - \mathcal{E}(\varepsilon, R, L, \rho)) \tag{13}$$

$$\text{Where:} \qquad (1 - \mathcal{E}(\varepsilon, R, L, \rho)) := (1-\varepsilon)\left(1 - \frac{1}{\rho L^3}\right)\left(1 - \frac{2R}{L}\right)^3\left(1 + \frac{4\pi\rho}{3}(R^3 - R_0^3)\right)^{-1} \times$$

$$\times \left(1 - \frac{\mathfrak{a}\left(\langle W_R^2 \rangle_{\Psi_0} - \langle W_R \rangle_{\Psi_0}^2\right)}{\langle W_R \rangle_{\Psi_0}\left(E_1^{(0)} - \mathfrak{a}\langle W_R \rangle_{\Psi_0}\right)}\right)\,. \tag{14}$$

Surely result (13) looks promising, but we still have two safety checks to make:

- the error $\mathcal{E}$ should be subleading with respect to $4\pi\rho\,\mathfrak{a}$;
- the use of Temple's inequality was a legitimate passage, i.e. $E_1^{(0)} - \mathfrak{a}\langle W_R\rangle_{\Psi_0} > 0$.

One could evaluate the error using (12) and the bound $\langle W_R^2\rangle_{\Psi_0} \leq \frac{3N}{R^3-R_0^3}\langle W_R\rangle_{\Psi_0}$ (that one can easily find by plugging in the definition of $W_R$, using $ab \leq (a^2+b^2)/2$ and the fact that $U_R(t_i)^2 = \frac{3}{R^2-R_0^2}U_R(t_i)$).

Unfortunately the second safety check fails. Recalling that $\Lambda$ has Neumann boundary conditions, then

$$E_1^{(0)} = \varepsilon\frac{\pi^2}{L^2}\,, \tag{15}$$

and using (12) one can show that

$$E_1^{(0)} - \mathfrak{a}\langle W_R\rangle_{\Psi_0} \leq \varepsilon\pi^2L^{-2} - 4\pi\rho^2\,\mathfrak{a}\,L^3 + (\text{subleading terms})\,,$$

a negative quantity for $L$ sufficiently large. Moreover this failure of the second safety check means that the error explodes for a certain length $L$, thus, $\mathcal{E}$ is not always subleading.

This means that our bound is not usable. But since the failure of Temple's inequality was due to how big $L$ was, we understand that this kind of technique works on small enough boxes. And this is the final and crucial idea: divide the Thermodynamic box $\Lambda$ in much smaller boxes with sidelength $\ell$ sufficiently small, that will be kept fixed in the limit $L \to \infty$. One uses this kind of bound on every little box and then sums all those contributions together.

The moral of the story is that the key for a good lower bound will be a good localization.

# 4 The actual bound

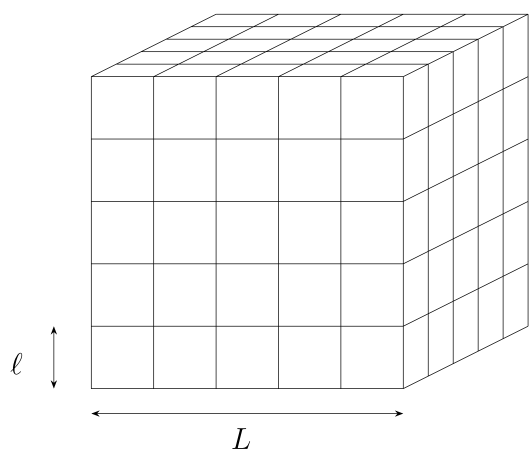


Figure 4: A big Neumann box, composed by many small Neumann boxes.

As briefly stated at the end of last section, we fix a length $\ell$, and we divide the thermodynamic box into smaller boxes $\Lambda_\ell$ with sidelength $\ell$. Let $M := \dfrac{L^3}{\ell^3} = \dfrac{N}{\rho\ell^3}$ be the total number of small boxes in which one is dividing $\Lambda$. We impose on each of these small boxes *Neumann* boundary conditions.

Even though the addition of this new constraint seems brutal, one has to remember that we are dealing with Bose gases. Physics tells us that most of the particles will be inside the Bose-Einstein condensate, represented by the constant wavefunction, and so imposing this boundary conditions on the small boxes only modifies the excited states, making what would usually be a brutal approximation rather gentle.

Then we distribute the $N$ particles inside those smaller boxes, compute the energy there and then sum together all those contributions. We note that we are neglecting the interaction between particles belonging to different cells and since $v \geq 0$ this lowers the energy.

Since the variational space in which we are choosing the minimum is now bigger (the boxes are now all independent from one another), in order to get a lower bound we minimize over all possible choices of the particle numbers for the various cells, with the constraint that the sum of the particle numbers in each cell must add up to $N$. Hence:

$$E_{GS}(N,L) \geq \inf_{\{n_i\}}\sum_{i=1}^{M} E_{GS}(n_i,\ell)\,, \tag{16}$$

where the infimum is taken over all possible configurations of numbers of particles in the boxes that respects the aforementioned constraint. Now let $m_n$ be the number of boxes with exactly $n$ particles inside of them. Then one can rewrite the above bound as:

$$E_{GS}(N,L) \geq \inf_{\{m_n\}}\sum_{n=0}^{N} m_nE_{GS}(n,\ell)\,, \tag{17}$$

where $\sum_{n=0}^{N} m_n = M$ and $\sum_{n=0}^{N} m_n n = N$.

From this last bound then one gets for the ground state energy per particle (noticing that $N = \rho\ell^3 M$):

$$\frac{E_{GS}(N,L)}{N} \geq (\rho\ell^3)^{-1} \inf_{\{m_n\}} \sum_{n=0}^{N} \frac{m_n}{M} E_{GS}(n,\ell) =: (\rho\ell^3)^{-1} \inf_{\{c_n\}} \sum_{n=0}^{N} c_n E_{GS}(n,\ell)\,, \tag{18}$$

where by construction, $\sum_{n=0}^{N} c_n = 1$ and $\sum_{n=0}^{N} n c_n = \rho\ell^3$.

A nice property of the ground state energy is **superadditivity**, i.e.

$$E_{GS}(n+\tilde{n},\ell) \geq E_{GS}(n,\ell) + E_{GS}(\tilde{n},\ell)\,. \tag{19}$$

Superadditivity follows immediately from the fact that $v \geq 0$: in fact it suffices to consider a cell with $n+\tilde{n}$ particles and to lower bound its energy by disregarding the interaction between the $n$ and the $\tilde{n}$ particles obtaining precisely (19).

A corollary of superadditivity will turn out extremely useful. Consider two integers $p, n$ with $n \geq p$, denoting by $\lfloor\cdot\rfloor$ the floor function, then one obtains:

$$E_{GS}(n,\ell) = E_{GS}\left(\left\lfloor\frac{n}{p}\right\rfloor p + r_{np}, \ell\right) \geq \left\lfloor\frac{n}{p}\right\rfloor E_{GS}(p,\ell) + E_{GS}(r_{np},\ell) \geq \frac{n}{2p} E_{GS}(p,\ell)\,, \tag{20}$$

where in the last passage we disregarded the positive term $E_{GS}(r_{np},\ell)$ and used the fact that for every integer $n \geq p$ it holds that $\lfloor n/p\rfloor \geq n/(2p)$.

Now we use (13) and (14), substituting $N$ with $n$, $L$ with $\ell$ and $\rho$ with $n/\ell^3$, thus obtaining:

$$\begin{aligned}
E_{GS}(n,\ell) \geq & 4\pi\frac{n^2}{\ell^3}\,\mathfrak{a}\left[(1-\varepsilon)\left(1-\frac{1}{n}\right)\left(1-\frac{2R}{\ell}\right)^3\left(1+\frac{4\pi n}{3\ell^3}(R^3-R_0^3)\right)^{-1}\times\right.\\
&\left.\times\left(1-\frac{\mathfrak{a}\left(\langle W_R^2\rangle_{\Psi_0}-\langle W_R\rangle_{\Psi_0}^2\right)}{\langle W_R\rangle_{\Psi_0}\left(E_1^{(0)}-\mathfrak{a}\langle W_R\rangle_{\Psi_0}\right)}\right)\right]\geq\\
\geq & \frac{4\pi n\,\mathfrak{a}}{\ell^3}(n-1)(1-\varepsilon)\left(1-\frac{2R}{\ell}\right)^3\left(1+\frac{4\pi n}{3\ell^3}(R^3-R_0^3)\right)^{-1}\times\\
&\times\left(1-\frac{\frac{3\,\mathfrak{a}\,n}{R^3-R_0^3}\langle W_R\rangle_{\Psi_0}-\mathfrak{a}\langle W_R\rangle_{\Psi_0}^2}{\langle W_R\rangle_{\Psi_0}\left(\varepsilon\pi^2\ell^{-2}-4\pi\,\mathfrak{a}\,\ell^{-3}n(n-1)\right)}\right)\geq\\
\geq & \frac{4\pi n\,\mathfrak{a}}{\ell^3}(n-1)(1-\varepsilon)\left(1-\frac{2R}{\ell}\right)^3\left(1+\frac{4\pi n}{3\ell^3}(R^3-R_0^3)\right)^{-1}\times\\
&\times\left(1-\frac{3\,\mathfrak{a}\,n}{\pi(R^3-R_0^3)\left(\varepsilon\pi\ell^{-2}-4\,\mathfrak{a}\,\ell^{-3}n(n-1)\right)}\right).
\end{aligned}$$

So, to summarize, one gets that:

$$E_{GS}(n,\ell) \geq \frac{4\pi n\,\mathfrak{a}}{\ell^3}(n-1)K(n,\ell)\,, \tag{21}$$

where:

$$\begin{aligned}
K(n,\ell) :=& (1-\varepsilon)\left(1-\frac{2R}{\ell}\right)^3\left(1+\frac{4\pi n}{3\ell^3}(R^3-R_0^3)\right)^{-1}\times\\
&\times\left(1-\frac{3\,\mathfrak{a}\,n}{\pi(R^3-R_0^3)\left(\varepsilon\pi\ell^{-2}-4\,\mathfrak{a}\,\ell^{-3}n(n-1)\right)}\right).
\end{aligned} \tag{22}$$

By the definition of $K(n,\ell)$ we see that such a function is monotonously decreasing in $n$. This means that for two integers $q$ and $n$ with $q \geq n$

$$E_{GS}(n,\ell) \geq \frac{4\pi n\,\mathfrak{a}}{\ell^3}(n-1)K(q,\ell)\,. \tag{23}$$

With this acquired knowledge we can look back at (18) and find, at fixed $p \in \{1, \ldots, N\}$:

$$\begin{aligned}\frac{E_{GS}(N,L)}{N} \geq& (\rho\ell^3)^{-1} \inf_{\{c_n\}} \sum_{n=0}^{N} c_n E_{GS}(n,\ell) = (\rho\ell^3)^{-1} \inf_{\{c_n\}} \left( \sum_{n=0}^{p-1} c_n E_{GS}(n,\ell) + \sum_{n=p}^{N} c_n E_{GS}(n,\ell) \right) \geq \\ &\geq (\rho\ell^3)^{-1} \inf_{\{c_n\}} \left( \sum_{n=0}^{p-1} c_n \frac{4\pi n\, \mathfrak{a}}{\ell^3}(n-1) K(p,\ell) + \sum_{n=p}^{N} c_n \frac{n}{2p} E_{GS}(p,\ell) \right) \geq \\ &\geq (\rho\ell^3)^{-1} \frac{4\pi\, \mathfrak{a}}{\ell^3} K(p,\ell) \inf_{\{c_n\}} \left( \sum_{n=0}^{p-1} c_n n(n-1) + \frac{1}{2} \sum_{n=p}^{N} c_n n(p-1) \right).\end{aligned} \tag{24}$$

What (24) tells us is that now our task is to minimize over all possible $\{c_n\}$ the expression:

$$\mathcal{M}_p[\{c_n\}] := \sum_{n=0}^{p-1} c_n n(n-1) + \frac{1}{2} \sum_{n=p}^{N} c_n n(p-1)\,. \tag{25}$$

We define $k := \rho\ell^3$ and $t_p := \sum_{n=0}^{p-1} c_n n \leq k = t_p[\{c_n\}]$. Noticing that one has that $\sum_{n=p}^{N} c_n n = k - t_p$ and that the function $n(n-1)$ is convex (this implies that its graph is all above its tangent line at 0) one finds that:

$$\mathcal{M}_p[\{c_n\}] \geq t_p(t_p - 1) + \frac{1}{2}(p-1)(k-t_p)\,. \tag{26}$$

So we can minimize the RHS of (26) for $0 \leq t_p \leq k$. So, if one chooses $p \geq 4k$ one can see that the minimum of the above expression is obtained at $t_p = k$ and it's equal to $k(k-1)$. Plugging this into (24) and choosing $p = 4k$ one gets:

$$\frac{E_{GS}(N,L)}{N} \geq (\rho\ell^3)^{-1} \frac{4\pi\, \mathfrak{a}}{\ell^3} K(4\rho\ell^3, \ell^3)\rho\ell^3(\rho\ell^3 - 1) = 4\pi\rho\, \mathfrak{a} \left(1 - \frac{1}{\rho\ell^3}\right) K(4\rho\ell^3, \ell)\,. \tag{27}$$

In order to finish the proof of the lower bound we need to choose the free parameters $\varepsilon, R$ and $\ell$ in a smart way. In order to do that we shall look at $K(4\rho\ell^3, \ell)$. Here, the diluteness hypothesis will be our best friend: the smallness of $\rho\, \mathfrak{a}^3$ will prove to be a useful tool.

$$\begin{aligned}K(4\rho\ell^3, \ell) \geq (1-\varepsilon)\left(1 - \frac{2R}{\ell}\right)^3 \left(1 + \frac{16\pi}{3}(\rho\, \mathfrak{a}^3)\left(\frac{\ell}{\mathfrak{a}}\right)^3 \left(\frac{R^3 - R_0^3}{\ell^3}\right)\right)^{-1} \times \\ \times \left(1 - \frac{12\pi(\rho\, \mathfrak{a}^3)}{\left(\frac{R^3 - R_0^3}{\ell^3}\right)\left(\varepsilon\pi^3 \left(\frac{\mathfrak{a}}{\ell}\right)^2 - 64\pi^2 \left(\frac{\ell}{\mathfrak{a}}\right)^3 (\rho\, \mathfrak{a}^3)^2\right)}\right),\end{aligned} \tag{28}$$

and moreover, one has that in terms of the diluteness parameter:

$$\left(1 - \frac{1}{\rho\ell^3}\right) = \left(1 - \left(\frac{\mathfrak{a}}{\ell}\right)^3 (\rho\, \mathfrak{a}^3)^{-1}\right).$$

We would like $K$ to be of the form (1− "Small stuff"), so a smart ansatz is to impose the following combinations of our free parameters to be powers of the diluteness parameter:

$$\varepsilon =: (\rho\, \mathfrak{a}^3)^{\alpha}\,, \qquad \frac{a}{\ell} =: (\rho\, \mathfrak{a}^3)^{\beta}\,, \qquad \frac{R^3 - R_0^3}{\ell^3} =: (\rho\, \mathfrak{a}^3)^{\gamma}\,. \tag{29}$$

In this way we reduce the choice of the parameters to a choice of the $\alpha, \beta, \gamma$ exponents. With these choices and noticing that $(2R/\ell) \sim (\rho\, \mathfrak{a}^3)^{\gamma/3}$ up to higher order terms, we have that the factor multiplying $4\pi\rho\, \mathfrak{a}$ in (27) is the following expression:

$$\left(1 - (\rho\, \mathfrak{a}^3)^{3\beta - 1}\right)\left(1 - (\rho\, \mathfrak{a}^3)^{\alpha}\right)\left(1 - C(\rho\, \mathfrak{a}^3)^{\gamma/3}\right)^3 \left(1 + \frac{16\pi}{3}(\rho\, \mathfrak{a}^3)^{1 - 3\beta + \gamma}\right)^{-1} \left(1 - 12\pi \frac{(\rho\, \mathfrak{a}^3)^{1-\gamma}}{\pi^3(\rho\, \mathfrak{a}^3)^{\alpha + 2\beta} - 64\pi^2(\rho\, \mathfrak{a}^3)^{2-3\beta}}\right). \tag{30}$$

where $C$ is an appropriate constant.

Looking at (30), we see that our exponents must satisfy the following conditions:

- The usage of Temple's inequality must be legitimate, hence

$$\pi^3(\rho\,\mathfrak{a}^3)^{\alpha+2\beta} - 64\pi^2(\rho\,\mathfrak{a}^3)^{2-3\beta} > 0\,,$$

  this means that the exponent on the left must be smaller than the one on the right (since $(\rho\,\mathfrak{a}^3) \ll 1$). This means that $2 > \alpha + 5\beta$.

- All the 5 factors must be of the form (1 − "Small stuff"), hence:

$$\begin{aligned} 3\beta - 1 &> 0\,; \\ \alpha &> 0\,; \\ \gamma &> 0\,; \\ 1 - 3\beta + \gamma &> 0\,; \\ 1 - \gamma - \alpha - 2\beta &> 0 \quad \text{(Assuming the validity of Temple inequality to hold true)}\,. \end{aligned}$$

One can choose for instance:

$$\alpha = \frac{1}{17}\,, \qquad \beta = \frac{6}{17}\,, \qquad \gamma = \frac{3}{17}\,,$$

and this would make all the conditions above satisfied. In the end this would amount to

$$\frac{E_{GS}(N,L)}{N} \geq 4\pi\rho\,\mathfrak{a}\left(1 - C(\rho\,\mathfrak{a}^3)^{1/17}\right)\,, \tag{31}$$

thus proving the leading order lower bound.

We remark that such a choice of exponents would amount (in the dilute regime) to:

$$\mathfrak{a} \ll R \ll \rho^{-1/3} \ll \ell \ll (\rho\,\mathfrak{a})^{-1/2}\,, \tag{32}$$

so, in order to achieve this lower bound, we need to localize on boxes with sides that are bigger than the interparticle distance, so that we have many particles in them, but smaller than the so called *healing length* $(\rho\,\mathfrak{a})^{-1/2}$, in order to preserve the spectral gap needed for Temple's inequality. QED

One can relax the hypothesis of $v$ having compact support, and substitute it with $v$ that decays at infinity faster that $1/r^3$ (necessary in order to have a well defined scattering length). In this case one proves the lower bound by approximating $v$ with compactly supported potentials, controlling the change in the scattering length.

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